8 2

30/05/2006

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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9	MAR 22	EMBASE is now updated on a daily basis
NEWS 10	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 11	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 12	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS 13	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 14	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 15	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 16	MAY 10	CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 17	MAY 11	KOREAPAT updates resume
NEWS 18	MAY 19	Derwent World Patents Index to be reloaded and enhanced

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
http://download.cas.org/express/v8.0-Discover/

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available after June 2006

Enter NEWS followed by the item number or name to see news on that specific topic.

* *

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Thank you in advance for your participation.

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FILE 'HOME' ENTERED AT 09:34:01 ON 30 MAY 2006

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:34:16 ON 30 MAY 2006
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STRUCTURE FILE UPDATES: 28 MAY 2006 HIGHEST RN 885861-83-6
DICTIONARY FILE UPDATES: 28 MAY 2006 HIGHEST RN 885861-83-6

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information

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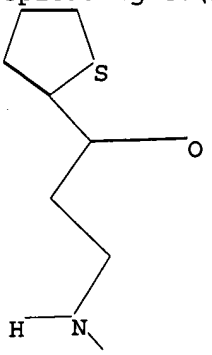
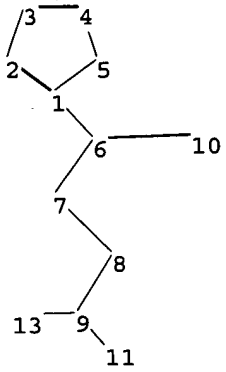
30/05/2006

on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10525820c.str





chain nodes :
6 7 8 9 10 11 13
ring nodes :
1 2 3 4 5
chain bonds :
1-6 6-7 6-10 7-8 8-9 9-11 9-13
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 6-10 8-9 9-11
exact bonds :
1-6 6-7 7-8 9-13

G1:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 13:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

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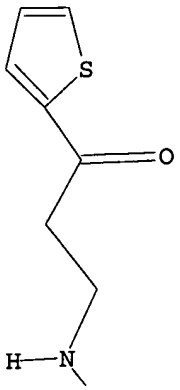

G1 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Ak

Structure attributes must be viewed using STN Express query preparation.

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=> s l1
SAMPLE SEARCH INITIATED 09:34:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      190 TO ITERATE

100.0% PROCESSED      190 ITERATIONS                                  9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         2973 TO     4627
PROJECTED ANSWERS:               9 TO      360

L2             9 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 09:34:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     4084 TO ITERATE

100.0% PROCESSED     4084 ITERATIONS                               100 ANSWERS
SEARCH TIME: 00.00.01

L3           100 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             166.94     167.15

FILE 'HCAPLUS' ENTERED AT 09:34:52 ON 30 MAY 2006
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FILE COVERS 1907 - 30 May 2006 VOL 144 ISS 23
FILE LAST UPDATED: 28 May 2006 (20060528/ED)

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This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3
L4 47 L3

=> save
ENTER L#, L# RANGE, ALL, OR (END):end

=> d ed abs ibib hitstr 1-47

L4 ANSWER 1 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 03 Feb 2006
AB A dosage form comprising of a high dose, high solubility active ingredient as modified release and a low dose active ingredient as immediate release where the weight ratio of immediate release active ingredient and modified release active ingredient is from 1:10 to 1:15000 and the weight of modified release active ingredient per unit is from 500 mg to 1500 mg; a process for preparing the dosage form. Tablets containing 10 mg sodium pravastatin and 1000 mg niacin were prepared The release of sodium pravastatin after 24 h was 67.7%, and the release of niacin after 1 h was 84.1%.

ACCESSION NUMBER: 2006:100738 HCAPLUS
DOCUMENT NUMBER: 144:198849
TITLE: Novel dosage form comprising modified-release and immediate-release active ingredients
INVENTOR(S): Vaya, Navin; Karan, Rajesh Singh; Sadanand, Sunil; Gupta, Vinod Kumar
PATENT ASSIGNEE(S): India
SOURCE: U.S. Pat. Appl. Publ., 49 pp., Cont.-in-part of U.S. Ser. No. 630,446.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2006024365	A1	20060202	US 2005-134633		20050519
US 2004096499	A1	20040520	US 2003-630446		20030729
PRIORITY APPLN. INFO.:			IN 2002-MU697	A	20020805
			IN 2002-MU699	A	20020805
			IN 2003-MU80	A	20030122
			IN 2003-MU82	A	20030122
			US 2003-630446	A2	20030729

IT **28745-68-8**, Thiofedrine
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel dosage form comprising modified-release and immediate-release

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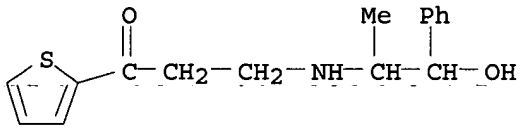
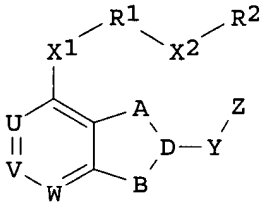
active ingredients)
RN 28745-68-8 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-(9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 24 Nov 2005
GI



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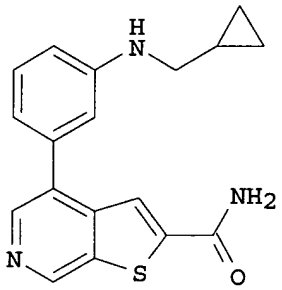


II

AB The invention is related to the preparation of fused heterocycles of formula I [A, B = independently N, S, O, a bond, etc.; D = C, N, S, O, C:C; U, V, W = independently CH and derivs., N; Y = a bond, CONH2 and derivs., SO, etc.; Z = H, halo, CN, etc.; X1 = a bond, halo, O, SO, NHSO2, etc.; R1 = a bond, (un)substituted benzofuranyl, benzimidazolyl, pyrrolyl, etc.; when R1 is not a bond, then X2 = a bond, O,S, NHCO and derivs., aliphatic group, etc.; or when R1 = a bond, then X2 = a bond and R2 is not a bond; R2 = a bond or (un)substituted benzoxazolyl, Ph, etc.; with provisos; and with the exception of certain compds.], and their pharmaceutically acceptable salts as inhibitors of kinases, particularly COT or MK2 kinases. The invention is also related to the use of certain compds. I as inhibitors of angiogenic receptor tyrosine kinases. Thus, reacting 4-(3-aminophenyl)thieno[2,3-c]pyridine-2-carboxamide with cyclopropanecarboxaldehyde gave thienopyridine II. All compds. I significantly inhibit either COT or MK2 at concns. of 50 μM or below.

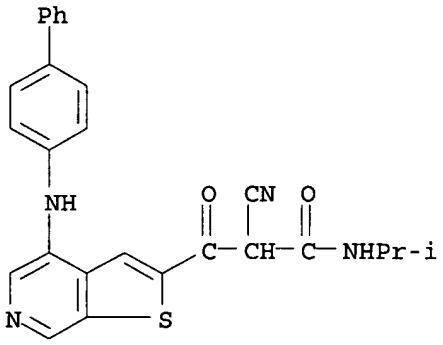
ACCESSION NUMBER: 2005:1240986 HCAPLUS
DOCUMENT NUMBER: 144:22906
TITLE: Preparation of fused heterocycle kinase inhibitors for treatment of protein tyrosine kinase-related diseases
INVENTOR(S): Cusack, Kevin; Salmeron-Garcia, Jose-Andres; Gordon, Thomas D.; Barberis, Claude E.; Allen, Hamish J.; Bischoff, Agniezka K.; Ericsson, Anna M.; Friedman, Michael M.; George, Dawn M.; Roth, Gregory P.; Talanian, Robert V.; Thomas, Christine; Wallace, Grier A.; Wishart, Neil; Yu, Zhengtian
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 362 pp.
CODEN: PIXXD2

30/05/2006

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005110410	A2	20051124	WO 2005-US16903	20050513
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2006074102	A1	20060406	US 2005-129624	20050513

PRIORITY APPLN. INFO.: US 2004-571281P P 20040514
OTHER SOURCE(S): MARPAT 144:22906
IT **870243-88-2P**, 3-[4-[(Biphenyl-4-yl)amino]thieno[2,3-c]pyridin-2-yl]-2-cyano-N-isopropyl-3-oxopropionamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(COT kinase inhibitor; preparation of fused heterocycles as kinase inhibitors)
RN 870243-88-2 HCAPLUS
CN Thieno[2,3-c]pyridine-2-propanamide, 4-([1,1'-biphenyl]-4-ylamino)-α-cyano-N-(1-methylethyl)-β-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 16 Sep 2005
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention discloses compds. I [R1 is H, OR8, NR9R10 or CHR9R10, where

R8, R9 and R10 are independently H, alkyl, aryl, cycloalkyl, etc; A, M are independently R, OR, NHR, NRR', SR, SO2R or halo; or A and M form a ring; E is CH or CR; L is CH, CR, CH2CR or CRCH2; R, R', R2, R3 are independently H, alkyl, cycloalkyl, aryl, heteroaryl, etc. or NRR' is heterocyclyl; Y is R4CR5R6-G-, where G is NH or O, R4 is alkyl, acyl, carbalkoxy, sulfamoyl, etc.; R5, R6 are independently H, alkyl, cycloalkyl, aryl, heteroaryl, etc.], including stereoisomers, pharmaceutically-acceptable salts or esters, etc., which have hepatitis C virus (HCV) protease inhibitory activity and includes methods for their synthesis and use in the treatment of disorders associated with the HCV protease. Synthetic examples and tables showing products of the invention along with Ki values are given. Thus, peptide II, prepared by a multistep procedure involving peptide coupling in solution, showed Ki = 5 nM for inhibition of HCV protease.

ACCESSION NUMBER: 2005:1004768 HCAPLUS
DOCUMENT NUMBER: 143:306546
TITLE: Preparation of peptides as inhibitors of hepatitis C virus NS3 protease
INVENTOR(S): Bogen, Stephane L.; Pan, Weidong; Ruan, Sumei; Chen, Kevin X.; Arasappan, Ashok; Venkatraman, Srikanth; Nair, Latha G.; Sannigrahi, Mousumi; Bennett, Frank; Saksena, Anil K.; Njoroge, F. George; Girijavallabhan, Viyyoor M.
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 570 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085275	A1	20050915	WO 2005-US6502	20050224
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005267043	A1	20051201	US 2005-65572	20050224

PRIORITY APPLN. INFO.: US 2004-548251P P 20040227
OTHER SOURCE(S): MARPAT 143:306546
IT **864802-67-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as inhibitors of hepatitis C virus NS3 protease)
RN 864802-67-5 HCAPLUS
CN 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-(cyclopropylmethyl)-2,3-dioxopropyl]-3-[(2S)-3,3-dimethyl-2-[[[[(1R)-1-(1-methylethyl)-3-oxo-3-(2-thienyl)propyl]amino]carbonyl]amino]-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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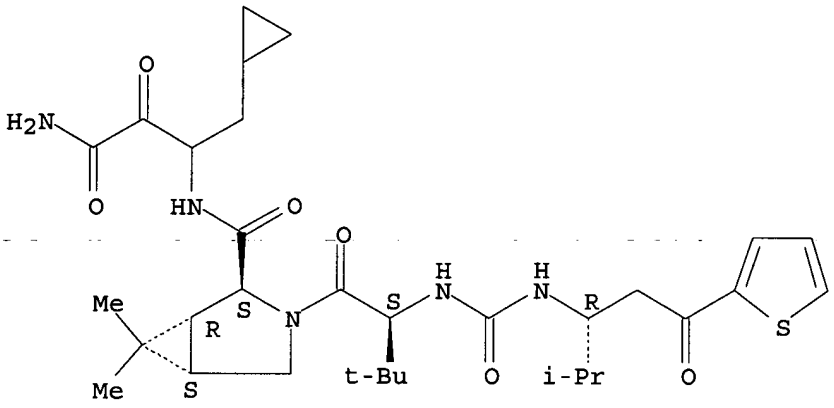
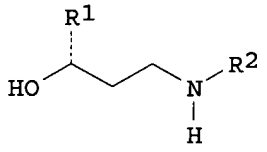


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 02 Sep 2005
GI



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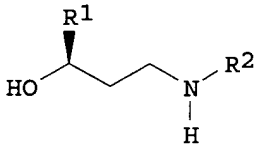

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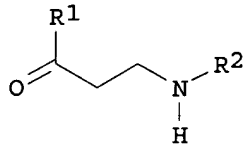

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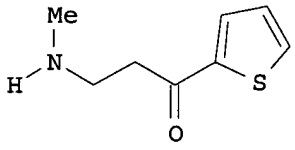
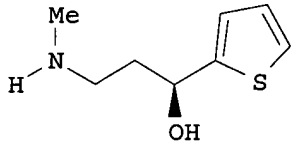


IV



V

AB A process for the preparation of enantiomerically pure 1-substituted-3-aminoalcs. of formula I [wherein R1 = (un)substituted 2-thienyl, (un)substituted 2-furanyl, or (un)substituted phenyl; R2 = (un)substituted C1-4 alkyl or (un)substituted phenyl] and formula II [wherein R1 = (un)substituted 2-thienyl, (un)substituted 2-furanyl, or (un)substituted phenyl; R2 = (un)substituted C1-4 alkyl or (un)substituted phenyl], by asym. hydrogenating an aminoketone or salts of a carboxylic acid and an aminoketone of formula III [wherein R1 = (un)substituted 2-thienyl, (un)substituted 2-furanyl, or (un)substituted phenyl; R2 = (un)substituted C1-4 alkyl or (un)substituted phenyl], and wherein the corresponding aminoalcs. are obtained by subsequent hydrolysis of their salts. Thus, a

mixture of 2-acetylthiophene, methylamine hydrochloride, and paraformaldehyde were heated to 120-130 °C for nine hours in ethanol and precipitated to provide 3-N-methylamino-1-(2-thienyl)-1 propanone hydrochloride (PRON-HCl, IV·HCl) which was subsequently stereoselectively reduced in the presence of a transition metal complex of a diphosphine ligand to provide (S)-(-)-3-N-methylamino-1-(2-thienyl)-1-propanol ((S)-PROL-HCl, V). Furthermore provided are salts of carboxylic acids with said aminoketones and the aminoalcs. obtained by asym. hydrogenating said aminoketones, resp.

ACCESSION NUMBER: 2005:962239 HCAPLUS
DOCUMENT NUMBER: 143:266590
TITLE: Process for the preparation of enantiomerically pure 1-substituted-3-aminoalcohols
INVENTOR(S): Michel, Dominique; Mettler, Hanspeter; McGarrity, John
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080370	A1	20050901	WO 2005-EP1781	20050221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1566383	A1	20050824	EP 2004-3809	20040219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: EP 2004-3809 A 20040219
EP 2004-10043 A 20040428

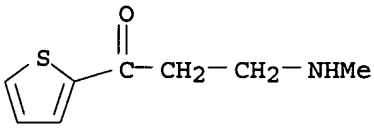
OTHER SOURCE(S): MARPAT 143:266590

IT **863094-06-8P 863094-15-9P 863094-23-9P 863094-31-9P**
RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the preparation of enantiomerically pure 1-substituted-3-aminoalcs.)

RN 863094-06-8 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with 3-(methylamino)-1-(2-thienyl)-1-propanone (1:1) (9CI) (CA INDEX NAME)

CM 1

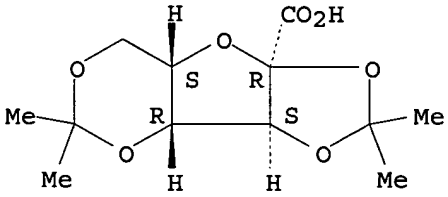
CRN 667465-15-8
CMF C8 H11 N O S



CM 2

CRN 18467-77-1
CMF C12 H18 O7

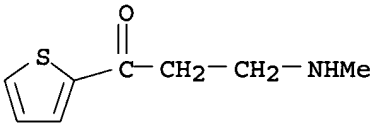
Absolute stereochemistry. Rotation (-).



RN 863094-15-9 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, benzoate (9CI) (CA INDEX NAME)

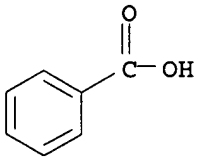
CM 1

CRN 667465-15-8
CMF C8 H11 N O S



CM 2

CRN 65-85-0
CMF C7 H6 O2

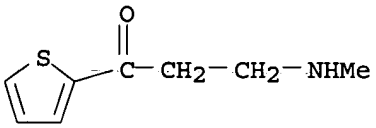


RN 863094-23-9 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

30/05/2006

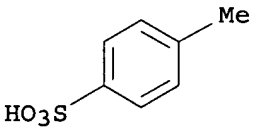
CM 1

CRN 667465-15-8
CMF C8 H11 N O S



CM 2

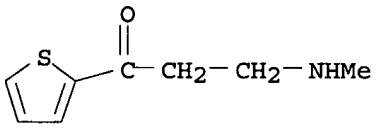
CRN 104-15-4
CMF C7 H8 O3 S



RN 863094-31-9 HCAPLUS
CN Dodecanoic acid, compd. with 3-(methylamino)-1-(2-thienyl)-1-propanone (1:1) (9CI) (CA INDEX NAME)

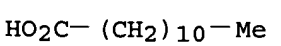
CM 1

CRN 667465-15-8
CMF C8 H11 N O S



CM 2

CRN 143-07-7
CMF C12 H24 O2

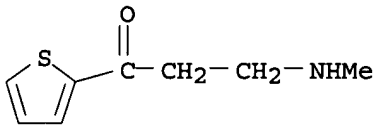


IT **645411-16-1P 863094-12-6P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the preparation of enantiomerically pure 1-substituted-3-aminoalcs.)
RN 645411-16-1 HCAPLUS

Young, Shawquia

30/05/2006

CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)

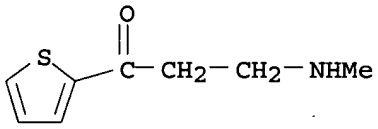


● HCl

RN 863094-12-6 HCAPLUS
CN L-xylo-2-Hexulosonic acid, compd. with 3-(methylamino)-1-(2-thienyl)-1-propanone (1:1) (9CI) (CA INDEX NAME)

CM 1

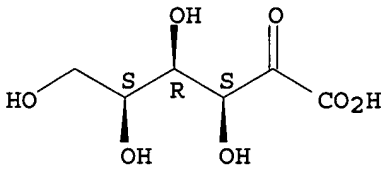
CRN 667465-15-8
CMF C8 H11 N O S



CM 2

CRN 526-98-7
CMF C6 H10 O7

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 26 Aug 2005
AB Provided is a process for the preparation of enantiomerically pure 1-substituted-3-amino alcs. (R)- or (S)-HOCH(R1)CH2CH2NHR2 (R1 = 2-thienyl, 2-furanyl, Ph, substituted 2-thienyl, substituted 2-furanyl, substituted Ph; R2 = C1-C4-alkyl, Ph, substituted C1-C4-alkyl, substituted Ph), particularly (S)-(-)- and (R)-(+)-3-N-methylamino-1-(2-thienyl)-1-propanol, by asym. hydrogenating salts of R1COCH2CH2NHR2 using Rh and an asym. ligand.

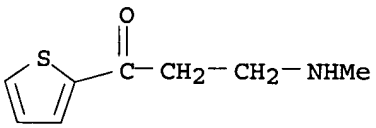
Young, Shawquia

30/05/2006

ACCESSION NUMBER: 2005:901934 HCAPLUS
DOCUMENT NUMBER: 143:248273
TITLE: Preparation of enantiomerically pure 1-substituted-3-amino alcohols
INVENTOR(S): Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: Eur. Pat. Appl., 14 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1566383	A1	20050824	EP 2004-3809	20040219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
WO 2005080370	A1	20050901	WO 2005-EP1781	20050221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: EP 2004-3809 A 20040219
EP 2004-10043 A 20040428
OTHER SOURCE(S): CASREACT 143:248273; MARPAT 143:248273
IT **645411-16-1P**, 3-(N-Methylamino)-1-(2-thienyl)-1-propanone hydrochloride **863094-06-8P 863094-15-9P 863094-23-9P 863094-31-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of 1-substituted -3-amino alcs. via hydrogenation of amino ketones)
RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



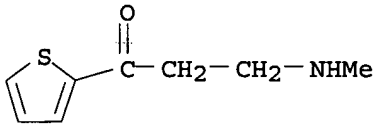
● HCl

RN 863094-06-8 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with 3-(methylamino)-1-(2-thienyl)-1-propanone (1:1) (9CI) (CA INDEX NAME)

Young, Shawquia

CM 1

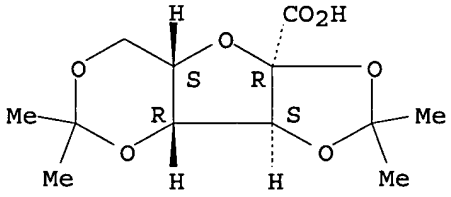
CRN 667465-15-8
CMF C8 H11 N O S



CM 2

CRN 18467-77-1
CMF C12 H18 O7

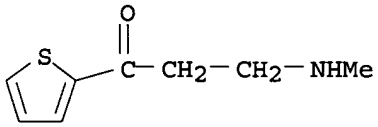
Absolute stereochemistry. Rotation (-).



RN 863094-15-9 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, benzoate (9CI) (CA INDEX NAME)

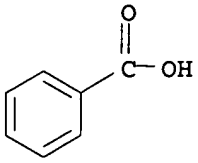
CM 1

CRN 667465-15-8
CMF C8 H11 N O S



CM 2

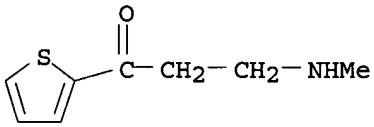
CRN 65-85-0
CMF C7 H6 O2



RN 863094-23-9 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

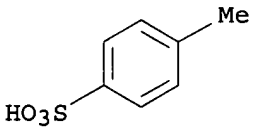
CM 1

CRN 667465-15-8
CMF C8 H11 N O S



CM 2

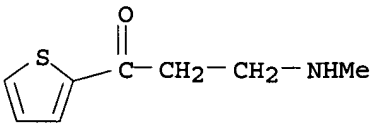
CRN 104-15-4
CMF C7 H8 O3 S



RN 863094-31-9 HCAPLUS
CN Dodecanoic acid, compd. with 3-(methylamino)-1-(2-thienyl)-1-propanone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 667465-15-8
CMF C8 H11 N O S



CM 2

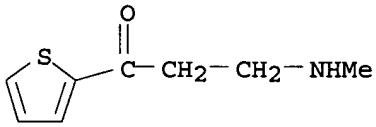
CRN 143-07-7
CMF C12 H24 O2

$HO_2C-(CH_2)_{10}-Me$

IT **863094-12-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of 1-substituted -3-amino alcs. via hydrogenation of amino ketones)
RN 863094-12-6 HCAPLUS
CN L-xylo-2-Hexulosonic acid, compd. with 3-(methylamino)-1-(2-thienyl)-1-propanone (1:1) (9CI) (CA INDEX NAME)

CM 1

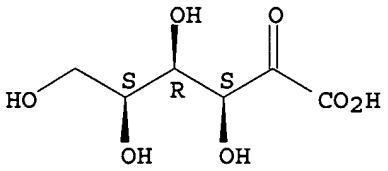
CRN 667465-15-8
CMF C8 H11 N O S



CM 2

CRN 526-98-7
CMF C6 H10 O7

Absolute stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 18 Jul 2005
AB The series of both syn- resp. anti-γ-thienyl-γ-hydroxy-α-aminobutanoic acids can be prepared using conjugate addition of chiral nonracemic 1-phenylethylamines on the corresponding β-thienoylacrylic acids and asym. reduction as the key steps of the synthesis. Raney nickel desulfurization in the hydrogen atmospheric represents straightforward access to the enantiomerically pure syn- resp. anti-γ-hydroxy-α-aminooctanoic resp. nonanoic acids derivs.
ACCESSION NUMBER: 2005:618404 HCAPLUS
DOCUMENT NUMBER: 144:253785
TITLE: Thienylsubstituted derivatives of α-aminobutanoic acid. Practical approach to

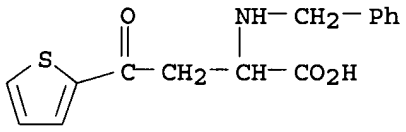
enantiomerically pure γ-hydroxy-α-aminooctanoic and γ-hydroxy-α-aminononanoic acids

AUTHOR(S): Berkes, Dusan; Gubala, Vladimir; Povazanec, Frantisek
CORPORATE SOURCE: Department of Organic Chemistry, Slovak Technical University, Bratislava, SK-812 37, Slovakia

SOURCE: International Electronic Conferences on Synthetic Organic Chemistry, 5th, 6th, Sept. 1-30, 2001 and 2002 [and] 7th, 8th, Nov. 1-30, 2003 and 2004 (2004), 1393-1404. Editor(s): Seijas, Julio A. Molecular Diversity Preservation International: Basel, Switz. CODEN: 69GTCO
DOCUMENT TYPE: Conference; (computer optical disk)
LANGUAGE: English

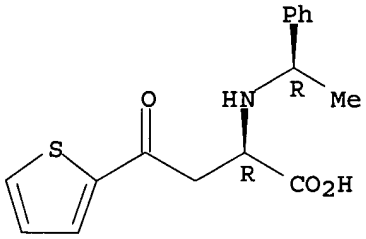
IT **204910-46-3P 877475-58-6P 877475-59-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of amino(thienyl)tetrahydrofuranones via Friedel-Crafts acylation of thiophenes with maleic anhydride followed by conjugate addition of amines, asym. reduction, and cyclization in the preparation of amino(hydroxy) acids)

RN 204910-46-3 HCAPLUS
CN 2-Thiophenebutanoic acid, γ-oxo-α-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



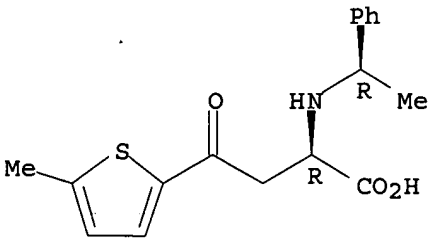
RN 877475-58-6 HCAPLUS
CN 2-Thiophenebutanoic acid, γ-oxo-α-[[(1R)-1-phenylethyl]amino]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



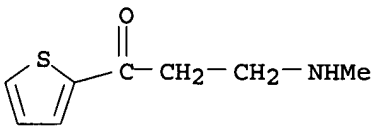
RN 877475-59-7 HCAPLUS
CN 2-Thiophenebutanoic acid, 5-methyl-γ-oxo-α-[[(1R)-1-phenylethyl]amino]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



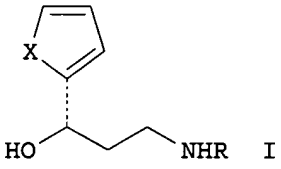
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 24 Mar 2005
AB Several β-secondary amino ketone hydrochlorides were hydrogenated with remarkably high enantioselectivities by using a rhodium complex containing P-chiral bisphospholane. These results establish a short and practical means for the synthesis of enantiopure N-monosubstituted γ-amino alcs., which are key intermediates in the synthesis of important antidepressants. For example, the bis[di(methyl)ethyl]tetra(hydro)-1,1'-bi-1H-isophosphindole-rhodium-catalyzed stereoselective hydrogenation of 3-(methylamino)-1-phenyl-1-propanone hydrochloride gave (αS)-α-[2-[(methyl)amino]ethyl]benzenemethanol, which is a synthetic precursor for (γS)-N-methyl-γ-[4-(trifluoromethyl)phenoxy]benzenepropanamine [i.e., (S)-fluoxetine]. The synthesis of (αS)-[-[(methyl)amino]ethyl]thiophenemethanol, a key synthetic intermediate for (S)-duloxetine, was also reported.
ACCESSION NUMBER: 2005:251916 HCAPLUS
DOCUMENT NUMBER: 142:481782
TITLE: Practical synthesis of enantiopure γ-amino alcohols by rhodium-catalyzed asymmetric hydrogenation of β-secondary-amino ketones
AUTHOR(S): Liu, Duan; Gao, Wenzhong; Wang, Chunjiang; Zhang, Xumu
CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Angewandte Chemie, International Edition (2005), 44(11), 1687-1689
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:481782
IT **645411-16-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral [(methyl)amino]ethyl]arenemethanol by bis[di(methyl)ethyl]tetra(hydro)-1,1'-bi-1H-isophosphindole-rhodium-catalyzed stereoselective hydrogenation using (aryl)[(methyl)amino]propanone hydrochloride as synthetic intermediate)
RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)

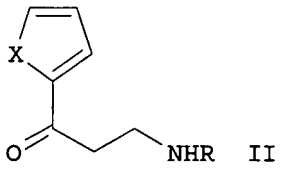


● HCl

L4 ANSWER 8 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 04 Mar 2005
GI



I



II

AB A process for the preparation of enantiomerically enriched or enantiomerically pure β-amino alcs. [I; X = S, O; R = (substituted) alkyl, cycloalkyl, aryl, aralkyl] comprises asym. hydrogenation of ketones (II; variables as above) using transition metal complexes of chiral bidentate phosphines as catalysts. Thus, 3-methylamino-1-(thien-2-yl)propan-1-one hydrochloride (preparation given), NaOMe, (S,S)-Me-DuPhos, and [Rh(COD)2]BF4 were autoclaved together in MeOH at 30-34° and 30 bar H2 for 5 h to give 67% (S)-3-methylamino-1-(2-thienyl)-1-propanol in >99% enantiomeric excess.

ACCESSION NUMBER: 2005:181066 HCAPLUS
DOCUMENT NUMBER: 142:280046
TITLE: Process for the asymmetric hydrogenation of β-amino ketones using transition metal complexes of chiral bidentate phosphines as catalysts.
PATENT ASSIGNEE(S): Lonza AG, Switz.
SOURCE: Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1510517	A1	20050302	EP 2003-77734	20030901
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004268057	A1	20050310	AU 2004-268057	20040831
WO 2005021527	A2	20050310	WO 2004-EP9690	20040831
WO 2005021527	A3	20050714		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,				

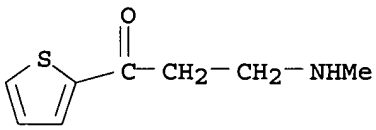
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

PRIORITY APPLN. INFO.: EP 2003-77734 A 20030901
WO 2004-EP9690 W 20040831

OTHER SOURCE(S): CASREACT 142:280046; MARPAT 142:280046

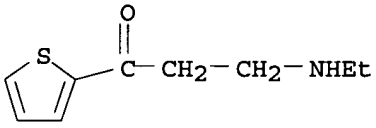
IT **645411-16-1P 645411-17-2P 645411-18-3P**
645411-19-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. hydrogenation of aminoketones using transition metal complexes of chiral bidentate phosphines as catalysts)

RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



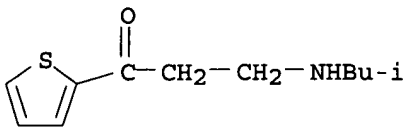
● HCl

RN 645411-17-2 HCAPLUS
CN 1-Propanone, 3-(ethylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



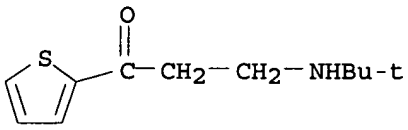
● HCl

RN 645411-18-3 HCAPLUS
CN 1-Propanone, 3-[(2-methylpropyl)amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 645411-19-4 HCAPLUS
CN 1-Propanone, 3-[(1,1-dimethylethyl)amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

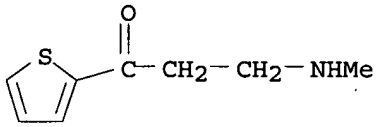
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 21 Oct 2004
AB The present invention concerns proteins, which possess an enzymic activity for reduction of substituted alkanones, such as 3-methylamino-1-(2-thienyl)-propane-1-one. Furthermore, the invention concerns nucleic acids which code for these proteins, vectors, and genetically modified microorganisms as well as procedures for the production of substituted (S)-alkanols, e.g., (S)-3-methylamino-1-(2-thienyl)-(S)-propanol. This compound may be used in the synthesis of duloxetine.
ACCESSION NUMBER: 2004:870926 HCAPLUS
DOCUMENT NUMBER: 141:348875
TITLE: L-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols
INVENTOR(S): Althoefer, Henning; Kesseler, Maria
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 41 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10315760	A1	20041021	DE 2003-10315760	20030407
CA 2521288	AA	20041021	CA 2004-2521288	20040406
WO 2004090094	A2	20041021	WO 2004-EP3655	20040406
WO 2004090094	A3	20050317		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1613745 A2 20060111 EP 2004-725924 20040406
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
CN 1771323 A 20060510 CN 2004-80009243 20040406
PRIORITY APPLN. INFO.: DE 2003-10315760 A 20030407
WO 2004-EP3655 W 20040406
OTHER SOURCE(S): CASREACT 141:348875
IT **667465-15-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(l-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols)
RN 667465-15-8 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)- (9CI) (CA INDEX NAME)

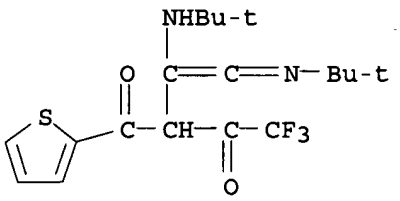


L4 ANSWER 10 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 29 Sep 2004
AB The 2:1 adducts produced in the reaction between Me3NC and RCOCH2COCF3 [R = Ph, 2-thienyl, 2-naphthyl] were isolated and characterized as fluorinated aminoketenimines Me3CN:C:C(NHCMe3)CH(COR)COCF3, which undergo enolization-cyclization reactions in boiling chloroform to produce new trifluoromethylated furan derivs.
ACCESSION NUMBER: 2004:792118 HCAPLUS
DOCUMENT NUMBER: 142:261346
TITLE: Reaction between tert-butyl isocyanide and 1,1,1-trifluoro-4-aryl-butane-2,4-diones. Synthesis of new trifluoromethylated furan derivatives
AUTHOR(S): Mosslemin, Mohammad H.; Yavari, Issa; Anary-Abbasinejad, Mohammad; Nateghi, Mohammad R.
CORPORATE SOURCE: Department of Chemistry, Islamic Azad University, Yazd, Iran
SOURCE: Journal of Fluorine Chemistry (2004), 125(10), 1497-1500
CODEN: JFLCAR; ISSN: 0022-1139
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:261346
IT **845965-02-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(reaction between tert-Bu isocyanide and 1,1,1-trifluoro-4-aryl-butane-2,4-diones to give trifluoromethylfuran derivs.)

RN 845965-02-8 HCAPLUS

CN 1,3-Butanedione, 2-[[(1,1-dimethylethyl)amino][(1,1-dimethylethyl)imino]ethenyl]-4,4,4-trifluoro-1-(2-thienyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 05 Aug 2004

AB New N-heteroarylcarbonylalanines of the D-series were stereoselectively prepared by stereoselective conjugate addition of benzylamine to enolates derived from D-mannitol. These compds. were active in binding and functional assays of the NMDA sub-type of glutamate receptors. (2R)-3-(2-Pyridinylcarbonyl)alanine inhibited MK801 binding, protected neurons from excitotoxic damage and blocked NMDA-induced currents in neurons. (2R)-3-(2-Thienylcarbonyl)alanine pos. modulated the NMDA receptor, possibly through the allosteric glycine site. described.

ACCESSION NUMBER: 2004:626166 HCAPLUS

DOCUMENT NUMBER: 141:296283

TITLE: Stereoselective synthesis and preliminary evaluation of new -3-heteroarylcarbonylalanines as ligands of the NMDA receptor

AUTHOR(S): Lima, Paulo G.; Caruso, Rodrigo R. B.; Alves, Simone O.; Pessoa, Renata F.; Mendonca-Silva, Dayde L.; Nunes, Ricardo J.; Noel, Francois; Castro, Newton G.; Costa, Paulo R. R.

CORPORATE SOURCE: Laboratorio de Quimica Bioorganica, Nucleo de Pesquisas de Produtos Naturais, Centro de Ciencias da Saude, Bloco J, Universidade Federal do Rio de Janeiro, Rio de Janeiro, 21941-590, Brazil

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(17), 4399-4403
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:296283

IT **764715-63-1P 764715-65-3P 764715-66-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

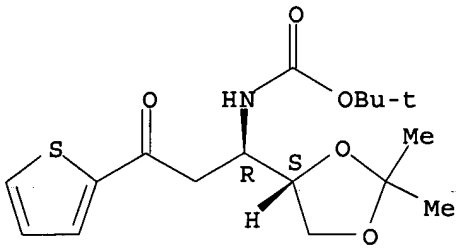
(asym. synthesis of heteroarylcarbonylalanines via stereoselective conjugate addition of benzylamine to enolate prepared from mannitol as NMDA receptor ligands)

RN 764715-63-1 HCAPLUS

CN Carbamic acid, [(1R)-1-[(4S)-2,2-dimethyl-1,3-dioxolan-4-yl]-3-oxo-3-(2-thienyl)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

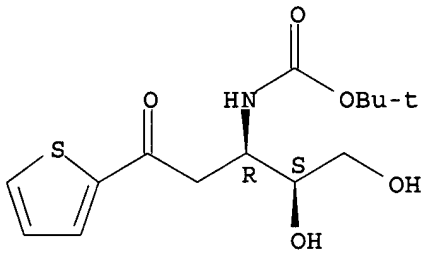
30/05/2006

Absolute stereochemistry.



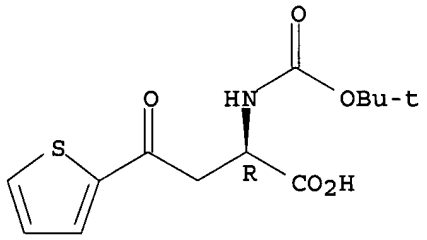
RN 764715-65-3 HCAPLUS
CN Carbamic acid, [(1R,2S)-2,3-dihydroxy-1-[2-oxo-2-(2-thienyl)ethyl]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 764715-66-4 HCAPLUS
CN 2-Thiophenebutanoic acid, α-[[(1,1-dimethylethoxy)carbonyl]amino]-γ-oxo-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 29 Jul 2004
AB 3-Methylamino-1-(2-thienyl)-1-propanone and its acid addition salts (e.g., the hydrochloride), which are useful as an intermediate in the production of the pharmaceutical (+)-(S)-N-methyl-3-(1-naphthyloxy)-3-(2-thienyl)propylamine oxalate (i.e., Duloxetine oxalate), are prepared
ACCESSION NUMBER: 2004:605494 HCAPLUS
DOCUMENT NUMBER: 141:140312
TITLE: 3-Methylamino-1-(2-thienyl)-1-propanone preparation and its use as a pharmaceutical intermediate

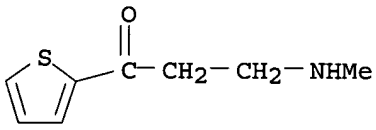
Young, Shawquia

30/05/2006

PATENT ASSIGNEE(S): BASF Ag, Germany
SOURCE: Ger. Offen., 4 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

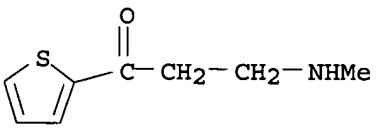
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10302595	A1	20040729	DE 2003-10302595	20030122
CA 2513542	AA	20040805	CA 2004-2513542	20040115
WO 2004065376	A1	20040805	WO 2004-EP237	20040115
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ				
EP 1587802	A1	20051026	EP 2004-702333	20040115
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1742003	A	20060301	CN 2004-80002686	20040115
PRIORITY APPLN. INFO.:			DE 2003-10302595 A	20030122
			WO 2004-EP237 W	20040115

IT **645411-16-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(3-methylamino-1-(2-thienyl)-1-propanone preparation and its use as a pharmaceutical intermediate)
RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



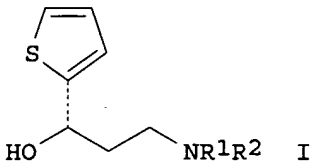
● HCl

IT **667465-15-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of)
RN 667465-15-8 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)- (9CI) (CA INDEX NAME)

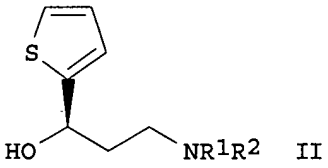


Young, Shawquia

L4 ANSWER 13 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 15 Apr 2004
GI



I



II

AB Title compds. (I, II; R1, R2 = H, alkyl, cycloalkyl, aralkyl, aryl), were prepared by reducing the corresponding 3-amino-1-(2-thienyl)-1-propanones using a hydrogen donor in the presence of a metal catalyst, an optically active N-containing ligand and optionally a base. Thus, 3-N-methylamino-1-(2-thienyl)-1-propanone hydrochloride (preparation given) and NaOH were stirred 1 h in Me2CHOH; a prestirred solution of (1S,2R)-cis-1-amino-2-indanol and (p-cymene)ruthenium(II)chloride dimer in Me2CHOH was added followed by stirring for 4 h at 20° to give 39% (S)-N-methylamino-1-(2-thienyl)-1-propanol in 70% enantiomeric excess.

ACCESSION NUMBER: 2004:308427 HCAPLUS
DOCUMENT NUMBER: 140:321232
TITLE: Preparation of optically active 3-amino-1-(2-thienyl)-1-propanols via reduction of 3-amino-1-(2-thienyl)-1-propanones using a hydrogen donor in the presence of a metal catalyst, an optically active nitrogen-containing ligand and optionally a base.
INVENTOR(S): Fuchs, Rudolf; Michel, Dominique; Brieden, Walter
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

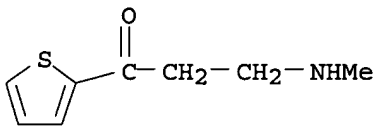
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031168	A2	20040415	WO 2003-EP11073	20031007
WO 2004031168	A3	20040826		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003276066	A1	20040423	AU 2003-276066	20031007

PRIORITY APPLN. INFO.: EP 2002-22540 A 20021007
WO 2003-EP11073 W 20031007
OTHER SOURCE(S): CASREACT 140:321232; MARPAT 140:321232

IT **645411-16-1P**, 3-N-Methylamino-1-(2-thienyl)-1-propanone hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of optically active aminothienylpropanols via reduction of aminothienylpropanones using a hydrogen donor in the presence of a metal catalyst, an optically active N-containing ligand and a base)

RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

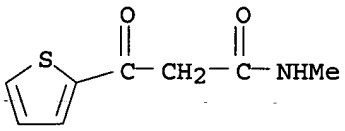
L4 ANSWER 14 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 08 Apr 2004
AB A process for the production of 3-heteroaryl-3-hydroxy-propionic acid derivs. by enantioselective microbial reduction is provided. Thus, Saccharomyces cerevisiae was used to reduce methyl-3-oxo-3-(2-thiophenyl)propanoic acid to methyl-(3S)-hydroxy-3-(2-thiophenyl)propanoic acid with a yield of 75% and an enantiomeric excess >97%. The reaction product then served as a reactant in the chemical synthesis of (1S)-3-(methylamino)-1-(2-thienyl)-1-propanol.

ACCESSION NUMBER: 2004:286808 HCAPLUS
DOCUMENT NUMBER: 140:302436
TITLE: Process for the production of 3-heteroaryl-3-hydroxy-propionic acid derivatives by enantioselective microbial reduction
INVENTOR(S): Berendes, Frank; Eckert, Markus; Brinkmann, Nils; Dreisbach, Claus; Meissner, Ruth; Koch, Rainhard
PATENT ASSIGNEE(S): Bayer Chemicals A.-G., Germany
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

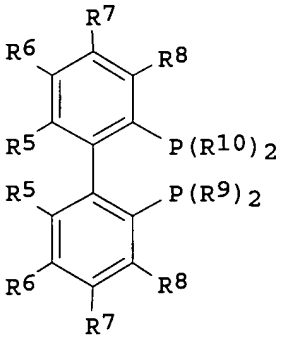
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1405917	A2	20040407	EP 2003-20847	20030913
EP 1405917	A3	20050112		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10244811	A1	20040408	DE 2002-10244811	20020926
US 2004181058	A1	20040916	US 2003-669424	20030924
JP 2004113245	A2	20040415	JP 2003-335690	20030926
CN 1497048	A	20040519	CN 2003-160307	20030926

PRIORITY APPLN. INFO.: DE 2002-10244811 A 20020926
OTHER SOURCE(S): MARPAT 140:302436
IT **603959-53-1**
RL: BCP (Biochemical process); BIOL (Biological study); PROC (Process)
(process for production of 3-heteroaryl-3-hydroxy-propionic acid derivs. by

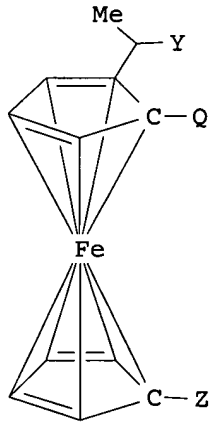
enantioselective microbial reduction)
RN 603959-53-1 HCAPLUS
CN 2-Thiophenepropanamide, N-methyl-β-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 15 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 14 Mar 2004
GI



I



II

AB The invention relates to methods for the enantioselective production of amino alcs., R1CH(OH)CH2(CH2)nNHR2 [R1 = (un)substituted, (un)saturated or aromatic carbocycle or heterocycle (optionally substituted with R3, R4); R2 = H, C1-20-alkyl; R3, R4 = H, C1-20-alkyl, C1-20-alkoxy, aryl, aryloxy, CO2R2, F, Cl, Br, OH, CN,NO2,N(R2)2, NHCOR2; n = 0 - 3], via the enantioselective hydrogenation of amino ketones, R1COCH2(CH2)nNHR2 and is characterized by hydrogenation in the presence of a non-racemic catalyst containing a chiral diphosphine ligand I [R5, R6, R7, R8 = H, C1-20-alkyl, C1-20-alkoxy, aryl, aryloxy, F, Cl, Br,N(R2)2, NHCOR2; R5R6, R6R7, R7R8 = (CH2)4, CH:CHCH:CH,etc.; R9, R10 = C6H4(R11)m, 2-furyl, cyclohexyl; R11 = H, C1-20-alkyl, C1-20-alkoxy, aryl, aryloxy, SO3Na, COR12, F, Cl, N(R12)2, NHCOR12; R12 = H, C1-20-alkyl; m = 0 - 3] or II [Q = PPh2, P(cyclohexyl)2, P[C6H3(CF3)2-3,5], P(4-methoxy-3,5-dimethylphenyl)2, P(CMe3)2; Y = OH, P(cyclohexyl)2, P(C6H3Me2-3,5)2, P(CMe3)2; Z = H, PPh2; Ph = unsubstituted Ph, C6H4Me-2, C6H4Me-3, C6H4Me-4, C6H3Me2]. Thus, (S)-N-methyl-3-hydroxy-3-(2-thienyl)propanamine was prepared with 92.8% e.e. from 3-(methylamino)-1-(2-thienyl)-1-propanone via asym. hydrogenation in MeOH/PhMe containing catalytic bis(1,5-cyclooctadiene)dirhodium(I) dichloride and (S)-(-)-2,2'-bis[di(p-tolyl)phosphine]-1,1'-binaphthyl.

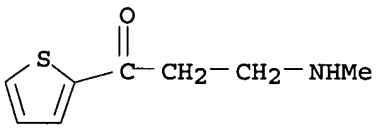
Young, Shawquia

30/05/2006

ACCESSION NUMBER: 2004:203795 HCAPLUS
DOCUMENT NUMBER: 140:253262
TITLE: Method for the preparation amino alcohols via the enantioselective hydrogenation of amino ketones
INVENTOR(S): Kralik, Joachim; Fabian, Kai; Muermann, Christoph; Schweickert, Norbert
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004020389	A1	20040311	WO 2003-EP8513	20030801
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2496883	AA	20040311	CA 2003-2496883	20030801
AU 2003260347	A1	20040319	AU 2003-260347	20030801
EP 1532100	A1	20050525	EP 2003-790842	20030801
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003013795	A	20050712	BR 2003-13795	20030801
CN 1678562	A	20051005	CN 2003-820304	20030801
JP 2005536556	T2	20051202	JP 2004-531845	20030801
US 2005261514	A1	20051124	US 2005-525821	20050225
ZA 2005002458	A	20051010	ZA 2005-2458	20050324
PRIORITY APPLN. INFO.:			DE 2002-10240025 A	20020827
			WO 2003-EP8513 W	20030801

OTHER SOURCE(S): CASREACT 140:253262; MARPAT 140:253262
IT **667465-15-8**, 3-(Methylamino)-1-(2-thienyl)-1-propanone
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective hydrogenation of; preparation amino alcs. via the enantioselective hydrogenation of amino ketones with chiral diphosphine ligands)
RN 667465-15-8 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN

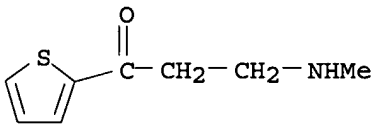
Young, Shawquia

30/05/2006

ED Entered STN: 11 Mar 2004
AB R1COCH2CH2NHR2 [R1 = (substituted) (unsatd.) residue, aromatic heterocyclyl; R2 = alkyl], were prepared by reaction of R1COCH2CH2NR2CH2CH2COR1 (variables as above) with R2NH2.
ACCESSION NUMBER: 2004:198214 HCAPLUS
DOCUMENT NUMBER: 140:235592
TITLE: Process for the preparation of monoalkylaminoethyl aryl ketones from bis(arylcarbonylethyl)alkylamines.
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: Ger. Offen., 7 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10240026	A1	20040311	DE 2002-10240026	20020827
CA 2497028	AA	20040311	CA 2003-2497028	20030801
WO 2004020391	A1	20040311	WO 2003-EP8514	20030801
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003260348	A1	20040319	AU 2003-260348	20030801
EP 1532101	A1	20050525	EP 2003-790843	20030801
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003013796	A	20050927	BR 2003-13796	20030801
CN 1678564	A	20051005	CN 2003-820305	20030801
JP 2005536557	T2	20051202	JP 2004-531846	20030801
PRIORITY APPLN. INFO.:			DE 2002-10240026 A	20020827
			WO 2003-EP8514 W	20030801

OTHER SOURCE(S): CASREACT 140:235592; MARPAT 140:235592
IT **667465-15-8P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of monoalkylaminoethyl aryl ketones from bis(arylcarbonylethyl)alkylamines)
RN 667465-15-8 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 17 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 18 Jan 2004

Young, Shawquia

30/05/2006

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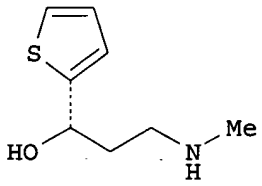

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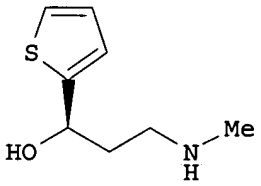

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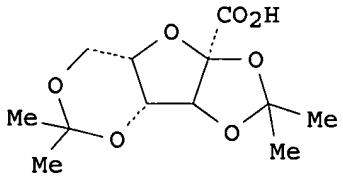
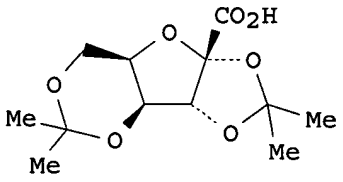


III



IV

AB Enantiomerically enriched (S)-(-)-3-N-methylamino-1-(2-thienyl)-1-propanol (I) or (R)-(+)-3-N-methylamino-1-(2-thienyl)-1-propanol (II) or mirror image are prepared by (i) treating an enantiomeric mixture of the amines I and II with (-)-2,3:4,6-di-O-isopropylidene-2-keto-L-gulonic acid (III) or (+)-2,3:4,6-di-O-isopropylidene-2-keto-D-gulonic acid (IV), (ii) crystallizing the obtained diastereomerically enriched salts from the reaction mixture obtained in step (i), (iii) optionally recrystg. said diastereomerically enriched salts I.III or II.IV, and (iv) treating the diastereomerically enriched salts II.III or II.IV obtained in step (ii) or step (iii) with a base to liberate the enantiomerically enriched amines I or II.

ACCESSION NUMBER: 2004:41488 HCAPLUS
DOCUMENT NUMBER: 140:93915
TITLE: Process for the preparation of optically active 3-N-methylamino-1-(2-thienyl)-1-propanol
INVENTOR(S): Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

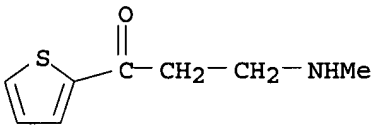
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005307	A1	20040115	WO 2003-EP7312	20030708
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003253036	A1	20040123	AU 2003-253036	20030708

PRIORITY APPLN. INFO.:
EP 2002-15161 A 20020709
WO 2003-EP7312 W 20030708

Young, Shawquia

30/05/2006

OTHER SOURCE(S): CASREACT 140:93915; MARPAT 140:93915
IT **645411-16-1P**, 3-(N-Methylamino)-1-(2-thienyl)-1-propanone hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of optically active N-methylamino(thienyl)propanol by optical resolution via formation of diastereomer salts with 2,3:4,6-di-O-isopropylidene-2-ketogulonic acid)
RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 18 Jan 2004
AB The invention relates to a process for the synthesis of N-monosubstituted β-amino alcs. of formula HOCH(R1)CH2CH2NHR2 and/or an addition salt of a proton acid (wherein R1 and R2 independently represent alkyl, cycloalkyl, aryl or aralkyl, each being optionally further substituted with alkyl, alkoxy and/or halogen) via direct preparation of N-monosubstituted β-amino ketones of R1COCH2CH2NHR2 and its addition salts of proton acids (wherein R1 and R2 are as defined above). Thus, 2-acetylthiophene 25.5, methylamine hydrochloride 14.9, paraformaldehyde 8.2, concentrated HCl 1.0 g, 100 mL ethanol were heated in an autoclave at 110° and a total pressure of 2-2.5 bar for 9 h, followed by removing 50 mL ethanol in vacuo and addition of 200 mL Et acetate under vigorous stirring, and filtration to give 71% 3-(methylamino)-1-(thiophen-2-yl)propan-1-one hydrochloride (I). To a mixture of 10.3 g I and 35 mL ethanol at 4° sodium hydroxide (4.0 g of a 50% aqueous solution) was added in about 5 min and afterwards, 0.95 g neat sodium borohydride in several portions in about 30 min. The resulting suspension was stirred for 4 h at the same temperature, treated dropwise with 10.0 mL acetone in 5 min, stirred for 10 addnl. minutes, treated with 20 mL H2O, concentrated about 5 times under vacuum, and extracted with tert-Bu Me ether (2 x 20 mL). The collected organic phases were finally concentrated under vacuum affording an orange oil which crystallized spontaneously after a few hours to give 3-(methylamino)-1-(thiophen-2-yl)propan-1-ol as an orange solid (7.2 g, 84 % yield).
ACCESSION NUMBER: 2004:41430 HCAPLUS
DOCUMENT NUMBER: 140:93914
TITLE: Process for the preparation of N-monosubstituted β-amino alcohols
INVENTOR(S): Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.

Young, Shawquia

30/05/2006

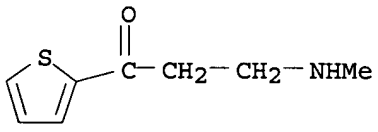
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005239	A1	20040115	WO 2003-EP7411	20030709
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2491472	AA	20040115	CA 2003-2491472	20030709
AU 2003250924	A1	20040123	AU 2003-250924	20030709
BR 2003012651	A	20050426	BR 2003-12651	20030709
EP 1539673	A1	20050615	EP 2003-762669	20030709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1665773	A	20050907	CN 2003-816223	20030709
JP 2005532383	T2	20051027	JP 2004-518758	20030709
NO 2005000079	A	20050311	NO 2005-79	20050106
US 2005256318	A1	20051117	US 2005-520362	20050418
PRIORITY APPLN. INFO.:			EP 2002-15229 A	20020709
			WO 2003-EP7411 W	20030709

OTHER SOURCE(S): CASREACT 140:93914; MARPAT 140:93914

IT **645411-16-1P**, 3-(Methylamino)-1-(thiophen-2-yl)propan-1-one hydrochloride **645411-17-2P**, 3-(Ethylamino)-1-(thiophen-2-yl)propan-1-one hydrochloride **645411-18-3P**, 3-(Isobutylamino)-1-(thiophen-2-yl)propan-1-one hydrochloride **645411-19-4P**, 3-(tert-Butylamino)-1-(thiophen-2-yl)propan-1-one hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for preparation of N-monosubstituted β-amino alcs. by reduction of N-monosubstituted β-amino ketones)

RN 645411-16-1 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)

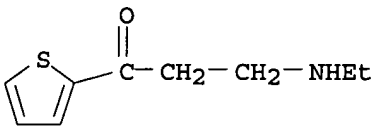


● HCl

RN 645411-17-2 HCAPLUS
CN 1-Propanone, 3-(ethylamino)-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX

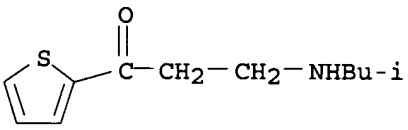
Young, Shawquia

NAME)



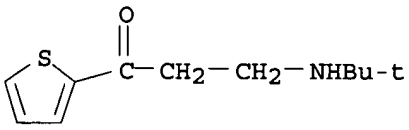
● HCl

RN 645411-18-3 HCAPLUS
CN 1-Propanone, 3-[(2-methylpropyl)amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 645411-19-4 HCAPLUS
CN 1-Propanone, 3-[(1,1-dimethylethyl)amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Dec 2003
AB The reactions of (S)-N-trifluoroacetyl-5-bromo-4-oxonorvaline Me ester with vicinal mercaptonitriles afforded δ-hetaryl-N-trifluoroacetyl-substituted α-amino acids (hetaryl is thiazol-2-yl, 2-thienyl, or thieno[2,3-b]pyridin-6-yl).
ACCESSION NUMBER: 2003:994927 HCAPLUS
DOCUMENT NUMBER: 140:287674
TITLE: Reactions of (S)-N-trifluoroacetyl-5-bromo-4-oxonorvaline methyl ester with vicinal mercaptonitriles. Synthesis of δ-hetaryl-

substituted α-amino acids

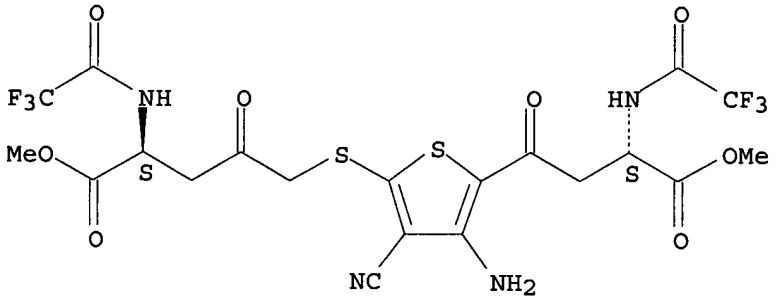
AUTHOR(S): Fedorov, A. E.; Shestopalov, A. M.; Belyakov, P. A.
CORPORATE SOURCE: N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, 119991, Russia

SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2003), 52(9), 2063-2069
CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER: Kluwer Academic/Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:287674

IT **676165-42-7P 676165-48-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of δ-heteroaryl α-amino acids from trifluoroacetylbromooxonorvaline and vicinal mercaptonitriles)

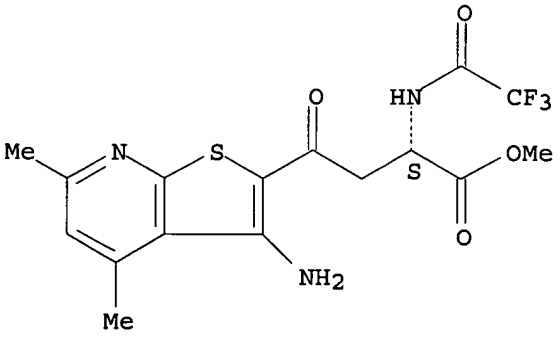
RN 676165-42-7 HCAPLUS
CN 2-Thiophenebutanoic acid, 3-amino-4-cyano-5-[[(4S)-5-methoxy-2,5-dioxo-4-[(trifluoroacetyl)amino]pentyl]thio]-γ-oxo-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 676165-48-3 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-4,6-dimethyl-γ-oxo-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



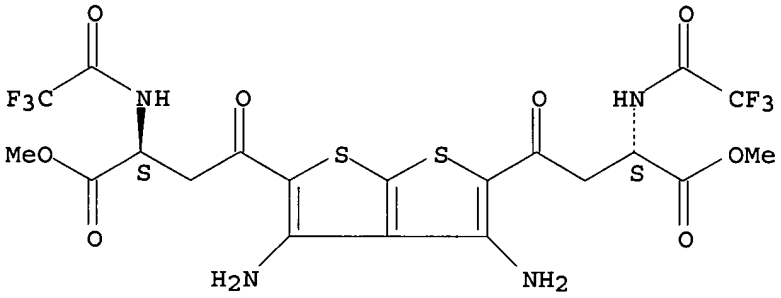
IT **676165-43-8P 676165-44-9P 676165-45-0P**

Young, Shawquia

676165-49-4P 676165-50-7P 676165-57-4P
676165-58-5P 676165-59-6P 676165-60-9P
676165-61-0P 676165-62-1P 676165-63-2P
676165-64-3P 676165-65-4P 676165-66-5P
676165-67-6P 676165-68-7P 676165-69-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of δ-heteroaryl α-amino acids from trifluoroacetylbromooxonorvaline and vicinal mercaptonitriles)

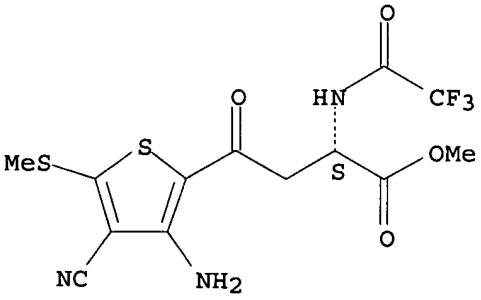
RN 676165-43-8 HCAPLUS
CN Thieno[2,3-b]thiophene-2,5-dibutanoic acid, 3,4-diamino-γ,γ'-dioxo-α,α'-bis[(trifluoroacetyl)amino]-, dimethyl ester, (αS,α'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



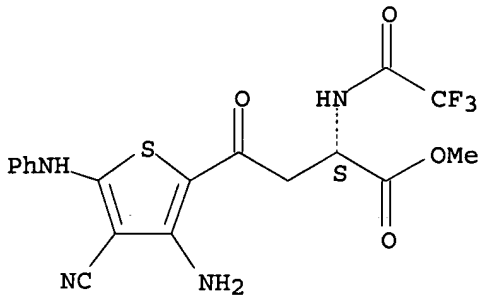
RN 676165-44-9 HCAPLUS
CN 2-Thiophenebutanoic acid, 3-amino-4-cyano-5-(methylthio)-γ-oxo-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



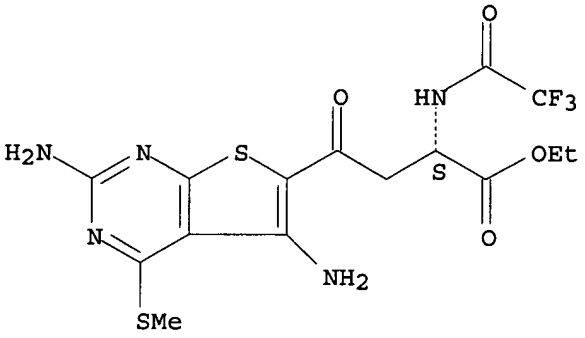
RN 676165-45-0 HCAPLUS
CN 2-Thiophenebutanoic acid, 3-amino-4-cyano-γ-oxo-5-(phenylamino)-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



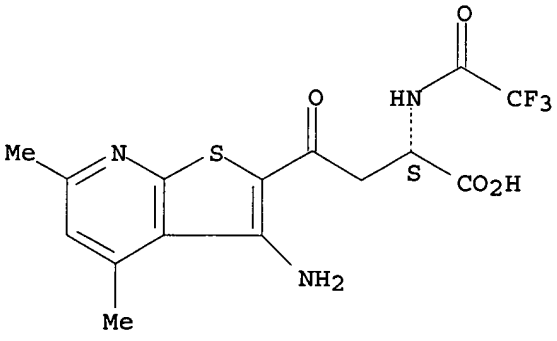
RN 676165-49-4 HCAPLUS
CN Thieno[2,3-d]pyrimidine-6-butanoic acid, 2,5-diamino-4-(methylthio)-γ-oxo-α-[(trifluoroacetyl)amino]-, ethyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676165-50-7 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-4,6-dimethyl-γ-oxo-α-[(trifluoroacetyl)amino]-, (αS)- (9CI) (CA INDEX NAME)

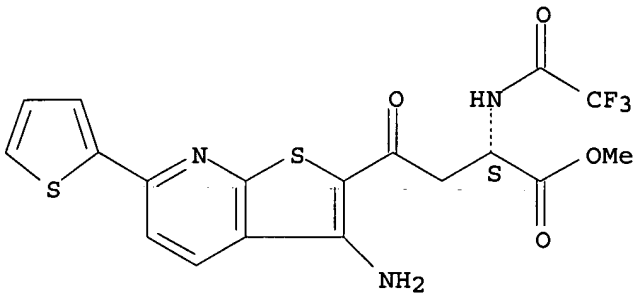
Absolute stereochemistry.



RN 676165-57-4 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-γ-oxo-6-(2-thienyl)-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

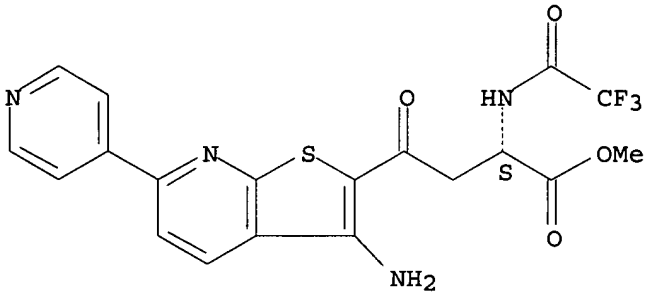
30/05/2006

Absolute stereochemistry.



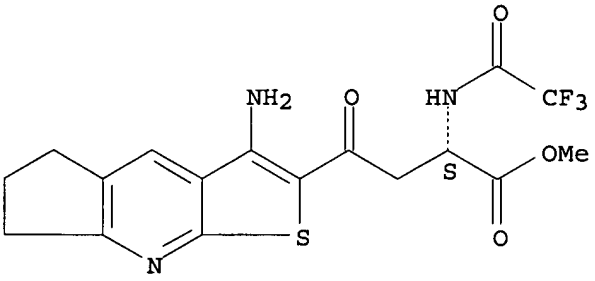
RN 676165-58-5 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-γ-oxo-6-(4-pyridinyl)-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676165-59-6 HCAPLUS
CN 5H-Cyclopenta[b]thieno[3,2-e]pyridine-2-butanoic acid, 3-amino-6,7-dihydro-γ-oxo-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676165-60-9 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-6-methyl-γ-oxo-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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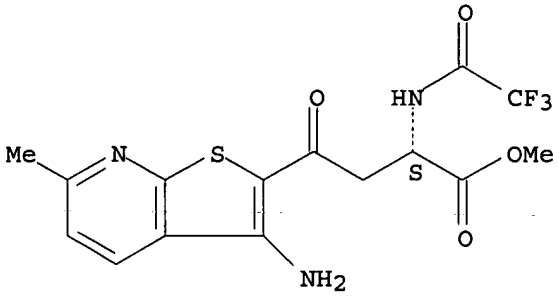
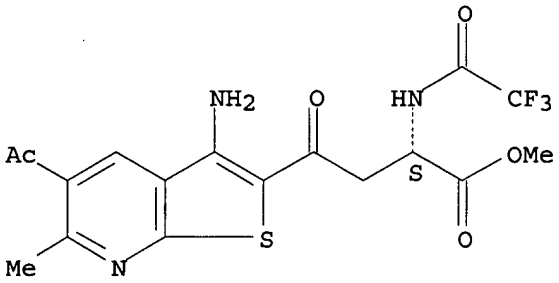


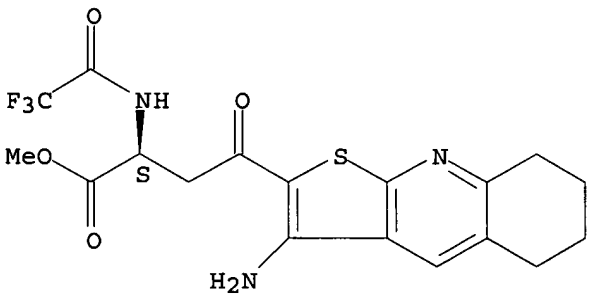
RN 676165-61-0 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 5-acetyl-3-amino-6-methyl-γ-oxo-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



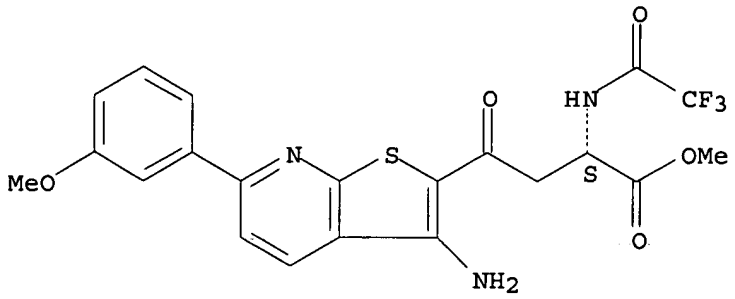
RN 676165-62-1 HCAPLUS
CN Thieno[2,3-b]quinoline-2-butanoic acid, 3-amino-5,6,7,8-tetrahydro-γ-oxo-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



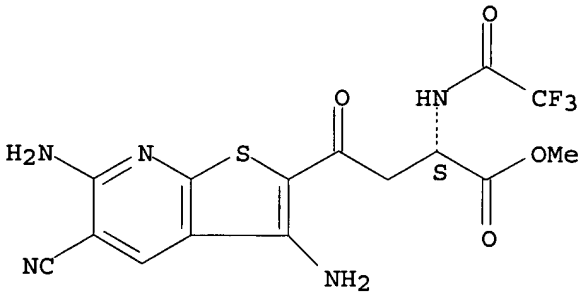
RN 676165-63-2 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-6-(3-methoxyphenyl)-γ-oxo-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



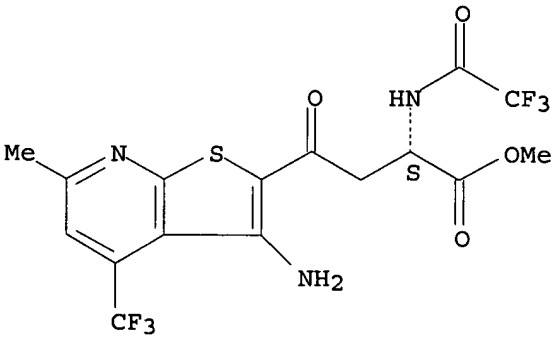
RN 676165-64-3 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3,6-diamino-5-cyano-γ-oxo-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



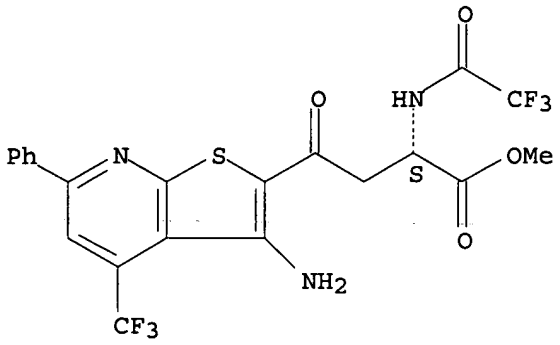
RN 676165-65-4 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-6-methyl-γ-oxo-α-[(trifluoroacetyl)amino]-4-(trifluoromethyl)-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



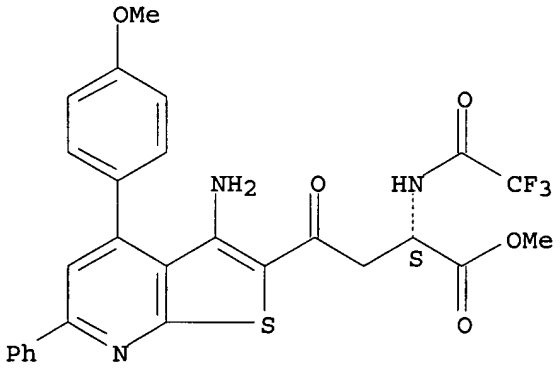
RN 676165-66-5 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-γ-oxo-6-phenyl-α-[(trifluoroacetyl)amino]-4-(trifluoromethyl)-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



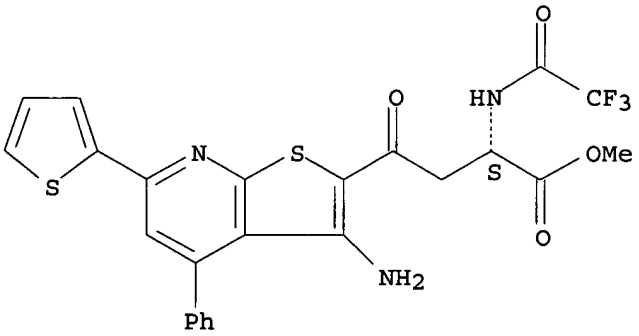
RN 676165-67-6 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-4-(4-methoxyphenyl)-γ-oxo-6-phenyl-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676165-68-7 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-γ-oxo-4-phenyl-6-(2-thienyl)-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676165-69-8 HCAPLUS
CN Thieno[2,3-b]pyridine-2-butanoic acid, 3-amino-4-(4-chlorophenyl)-γ-

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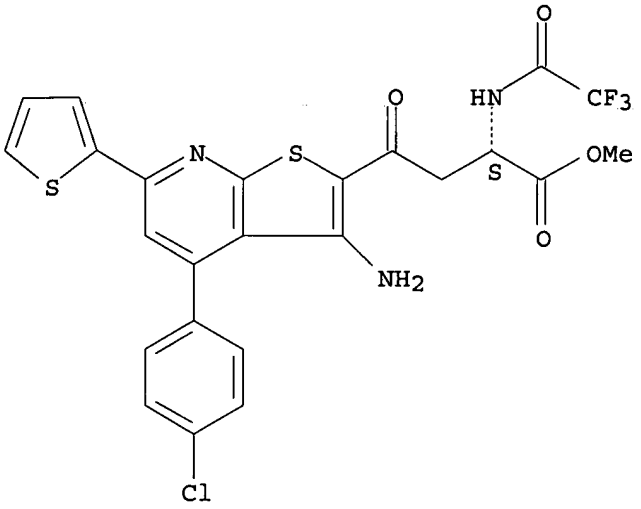
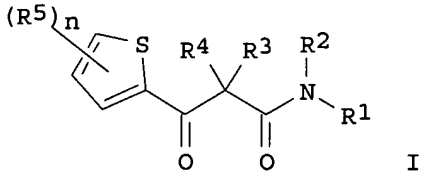
oxo-6-(2-thienyl)-α-[(trifluoroacetyl)amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 26 Sep 2003
GI



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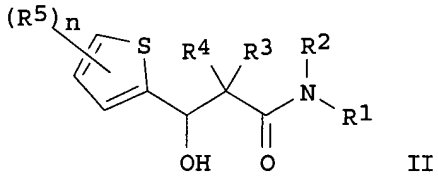

II

AB This invention pertains to a method for producing 3-oxo-3-(2-thienyl)propionamides with general formula of I [wherein R1 and R2 = independently H, alkyl, aryl, or aralkyl; R3 and R4 = independently H or alkyl; or R3 and R4 together form a ring with the nitrogen atom attached; R5 = halo, NO2, OH, (un)substituted alkyl, aryl, or alkoxy; n = 0-3] and a process for industrially producing optically active 3-amino-1-(2-thienyl)-1-propanol derivs. with general formula of II at low cost from the propionamides in high yields with high optical purity. The process comprises subjecting a β-ketocarbonyl compound having a thiophene ring to asym. reduction either in the presence of a catalyst comprising a compound of a Group 8 or 9 metal of the Periodic Table (e.g., ruthenium compound) and an asym. ligand (e.g., diphenylethylenediamine derivative) or using cells of a microorganism. Thus, 2-acetylthiophene was treated with NaH in THF, followed by the addition of di-Et carbonate to give 3-oxo-3-(2-thienyl)propionic acid Et ester (74%). The ester was treated with HCO2H in DMF in the presence of SS-TsDPEN and Et3N to provide (S)-3-hydroxy-3-(2-thienyl)propionic acid Et ester (94%) with 97.5% e.e.

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The chiral ester was treated with MeNH2 in MeOH to afford (S)-3-hydroxy-N-methyl-3-(2-thienyl)propionamide (93%) with 99% e.e.

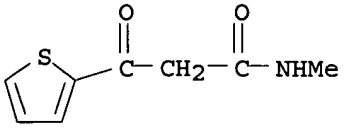
ACCESSION NUMBER: 2003:757695 HCAPLUS
DOCUMENT NUMBER: 139:261165
TITLE: Process for preparation of 3-hydroxy-3-(2-thienyl)propionamide derivatives
INVENTOR(S): Takehara, Jun; Qu, Jingping; Kanno, Kazuaki; Kawabata, Hiroshi; Dekishima, Yasumasa; Ueda, Makoto; Endo, Kyoko; Murakami, Takeshi; Sasaki, Tomoko; Uehara, Hisatoshi; Matsumoto, Youichi; Suzuki, Shihomi
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003078418	A1	20030925	WO 2003-JP3170	20030317
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2003335732	A2	20031128	JP 2002-141145	20020516
JP 2004067559	A2	20040304	JP 2002-227401	20020805
JP 2004067560	A2	20040304	JP 2002-227402	20020805
JP 2004067577	A2	20040304	JP 2002-228495	20020806
JP 2003342275	A2	20031203	JP 2002-317857	20021031
AU 2003221028	A1	20030929	AU 2003-221028	20030317
EP 1486493	A1	20041215	EP 2003-712723	20030317
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004155756	A2	20040603	JP 2003-102914	20030407
US 2005107621	A1	20050519	US 2004-944055	20040920

PRIORITY APPLN. INFO.:

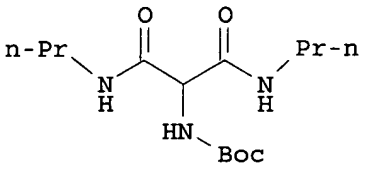
JP 2002-76168	A	20020319
JP 2002-129140	A	20020430
JP 2002-141145	A	20020516
JP 2002-227401	A	20020805
JP 2002-227402	A	20020805
JP 2002-228495	A	20020806
JP 2002-267617	A	20020913
JP 2002-317857	A	20021031
WO 2003-JP3170	W	20030317

OTHER SOURCE(S): MARPAT 139:261165
IT **603959-53-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hydroxy(thienyl)propionamide derivs.)
RN 603959-53-1 HCAPLUS
CN 2-Thiophenepropanamide, N-methyl-β-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 06 Dec 2002
GI



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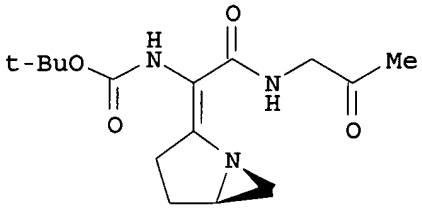
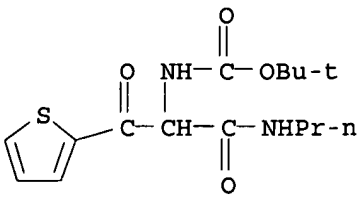


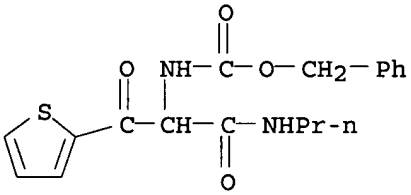
II

AB Condensation of acid chlorides (alkyl, aryl or heteroaryl) with N,N'-dialkyl α-acylamino malonamides in the presence of magnesium ethoxide provides a direct route to α-acylamino-β-keto amides, e.g. I, in moderate to good yields (46-95%). Using this method, a concise route to an enantiomerically enriched 1-azabicyclo[3.1.0]hexane II containing most of the elements of the right-hand' domain of azinomycin A has been developed.

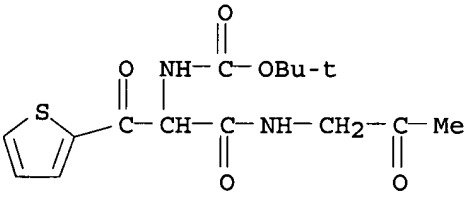
ACCESSION NUMBER: 2002:924950 HCAPLUS
DOCUMENT NUMBER: 138:204852
TITLE: Concise route to α-acylamino-β-keto amides: application to the synthesis of a simplified azinomycin A analogue
AUTHOR(S): Goujon, Jean-Yves; Shipman, Michael
CORPORATE SOURCE: School of Chemistry, University of Exeter, Exeter, EX4 4QD, UK
SOURCE: Tetrahedron Letters (2002), 43(52), 9573-9576
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:204852
IT **500109-23-9P 500109-26-2P 500109-29-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of α-acylamino-β-keto amides and a simplified azinomycin A analog)
RN 500109-23-9 HCAPLUS
CN Carbamic acid, [2-oxo-1-[(propylamino)carbonyl]-2-(2-thienyl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 500109-26-2 HCAPLUS
CN Carbamic acid, [2-oxo-1-[(propylamino)carbonyl]-2-(2-thienyl)ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 500109-29-5 HCAPLUS
CN Carbamic acid, [2-oxo-1-[[(2-oxopropyl)amino]carbonyl]-2-(2-thienyl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



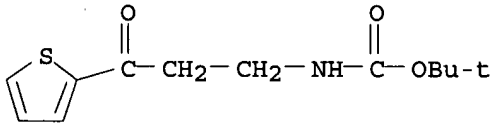
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 09 May 2001
AB 2-Lithiothiophene and 2-lithiopyridine were allowed to react with N-substituted β-amino esters RR1NCHRCO2Me [R = H, CH2Ph; R1 = H, BOC; R2 = H, 2,2-dimethyl-1,3-dioxolan-4-yl]. Only β-amino aryl ketones were obtained from N-BOC-N-H derivs., while aryl enoates were formed (retro-conjugate addition) from those substrates bearing N-Bn, N-H substituents, despite the aryllithium used. When the nitrogen is disubstituted (BOC and Bn), the product distribution depended on the nucleophile, leading to tertiary alcs. for 2-lithiothiophene or ketones for 2-lithiopyridine. Tertiary alcs. were also formed when PhLi was used as a nucleophile.
ACCESSION NUMBER: 2001:330712 HCAPLUS
DOCUMENT NUMBER: 135:137374
TITLE: Synthesis of β-amino aryl ketones through the addition of ArLi derivatives to β-amino esters
AUTHOR(S): Lima, P. G.; Sequeira, L. C.; Costa, P. R. R.
CORPORATE SOURCE: Nucleo de Pesquisas de Produtos Naturais, Laboratorio de Quimica Bioorganica (LQB), Universidade Federal do

Rio de Janeiro (UFRJ), Rio de Janeiro, 21941-590, Brazil
SOURCE: Tetrahedron Letters (2001), 42(21), 3525-3527
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:137374

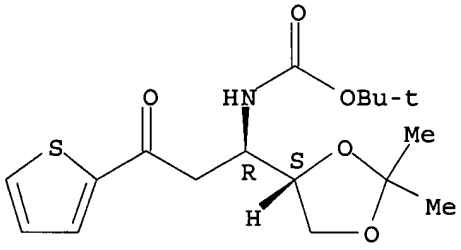
IT **351901-55-8P 351901-56-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of β-amino aryl ketones through the addition of aryllithium derivs. to β-amino esters)

RN 351901-55-8 HCAPLUS
CN Carbamic acid, [3-oxo-3-(2-thienyl)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 351901-56-9 HCAPLUS
CN threo-Pentose, 2,3-dideoxy-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,5-O-(1-methylethylidene)-1-C-2-thienyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



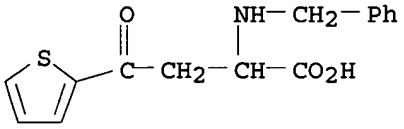
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 13 Jul 2000
AB A highly stereoselective reduction of γ-oxo-α-amino acids by sodium borohydride in the presence of a catalytic amount of manganese(II) chloride gives syn-γ-hydroxy-α-amino acids. Enantiomerically pure syn-(2S,4R,1'S)-4-aryl-4-hydroxy-2-(1'-phenylethylamino)butanoic acids form stable gels in methanol.

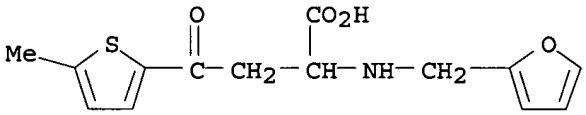
ACCESSION NUMBER: 2000:471573 HCAPLUS
DOCUMENT NUMBER: 133:238268
TITLE: Stereoselective sodium borohydride reduction, catalyzed by manganese(II) chloride, of γ-oxo-α-amino acids. A practical approach to syn-γ-hydroxy-α-amino acids
AUTHOR(S): Berkes, Dusan; Kolarovic, Andrej; Povazanec, Frantisek
CORPORATE SOURCE: Department of Organic Chemistry, Slovak Technical University, Bratislava, SK-812 37, Slovakia

30/05/2006

SOURCE: Tetrahedron Letters (2000), 41(27), 5257-5260
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:238268
IT **204910-46-3P 293309-47-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of syn-γ-hydroxo-α-amino acids by stereoselective sodium borohydride reduction of γ-oxo-α-amino acids catalyzed by manganese(II) chloride)
RN 204910-46-3 HCAPLUS
CN 2-Thiophenebutanoic acid, γ-oxo-α-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 293309-47-4 HCAPLUS
CN 2-Thiophenebutanoic acid, α-[(2-furanylmethyl)amino]-5-methyl-γ-oxo- (9CI) (CA INDEX NAME)



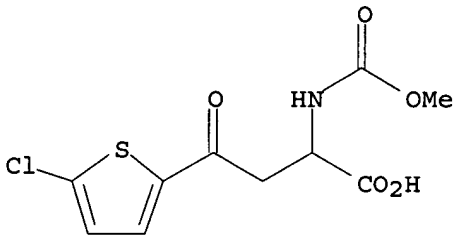
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 19 Jan 1999
AB Several N-protected 4-aryl-2-aminobutanoic and 5-aryl-2-aminopentanoic acids were prepared in good yields by reduction of the corresponding aromatic or heteroarom. ketones [e.g., p-ClC6H4CO(CH2)nCH(NHCO2Me)CO2H (n = 1 or 2)] with Et3SiH or PhMe2SiH in the presence of TiC14, resp. The reduction proceeded without racemization and was successfully applied to the synthesis of optically active γ- and δ-aryl substituted amino acids (R)- or (S)-p-ClC6H4CH2(CH2)nCH(NH2)CO2H.
ACCESSION NUMBER: 1999:32687 HCAPLUS
DOCUMENT NUMBER: 130:153943
TITLE: New silane reduction of aromatic ketones mediated by titanium tetrachloride: A synthesis of γ- and δ-aryl substituted amino acids
AUTHOR(S): Yato, Michihisa; Homma, Koichi; Ishida, Akihiko
CORPORATE SOURCE: Medicinal Chemistry Research Laboratory, Tanabe Seiyaku Co., Ltd., Toda, Saitama, 335, Japan
SOURCE: Heterocycles (1998), 49, 233-254
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal

Young, Shawquia

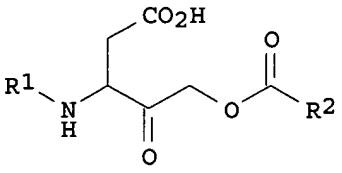
30/05/2006

LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:153943
IT **166764-45-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of aryl amino acids by silane reduction of aromatic ketones mediated by titanium tetrachloride)
RN 166764-45-0 HCAPLUS
CN 2-Thiophenebutanoic acid, 5-chloro-α-[(methoxycarbonyl)amino]-γ-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 25 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 02 May 1998
GI



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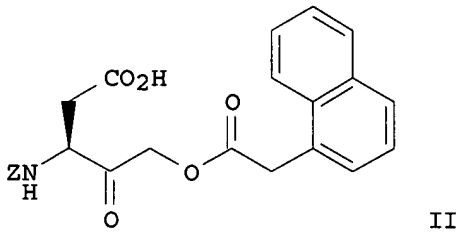


II

AB The present invention relates to compds. I [R1 = carboxy, acyl, amino acid residue, etc.; R2 = (CR2)n-X-R3; each R = independently H, C1-6 alkyl, OH; R3 = (un)substituted aryl, (un)substituted heteroaryl, (un)substituted heterocyclyl, cycloalkyl, etc; X = bond, O, S; n = 0-3; and the pharmaceutically acceptable salts, esters, amides, and prodrugs thereof] as inhibitors of interleukin-1β converting enzyme (ICE). This invention also relates to a method of treatment of stroke, inflammatory diseases, reperfusion injury, Alzheimer's disease, and shigellosis, and to a pharmaceutically acceptable composition that contains a compound that is an inhibitor of interleukin-1β converting enzyme. Thus, substitution of Z-Asp(OCMe3)-CH2Br (Z = PhCH2O2C) with 1-naphthylacetic acid, followed by acidic deprotection, gave desired aspartate ester derivative II. II inhibited ICE with Ki = 0.460 μM and IC50 = 3.100 μM, and inhibited Ich-2 (caspase-4) with IC50 = 3.60 μM, as determined using in vitro assays. Related prepared compds. I (196 examples) were also tested for ICE inhibition (Ki values of 0.00008 to 76 μM and IC50 values of 0.0013 to

32 μM), and Ich-2 inhibition (IC50 = 0.021 to 76 μM).

ACCESSION NUMBER: 1998:251152 HCAPLUS
DOCUMENT NUMBER: 128:321926
TITLE: Preparation of aspartate ester inhibitors of interleukin-1β converting enzyme
INVENTOR(S): Albrecht, Hans P.; Allen, Hamish John; Brady, Kenneth Dale; Caprathe, Bradley William; Gilmore, John Lodge; Harter, William Glen; Hays, Sheryl Jeanne; Kostlan, Catherine Rose; Lunney, Elizabeth Ann; Para, Kimberly Suzanne; et al.
PATENT ASSIGNEE(S): Warner-Lambert Company, USA
SOURCE: PCT Int. Appl., 179 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

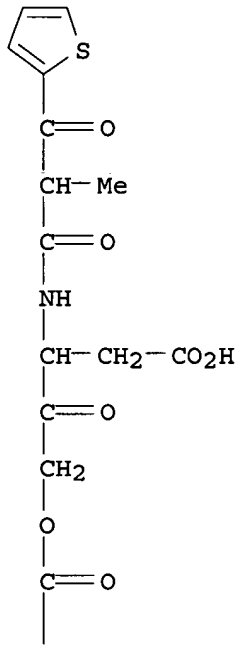
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9816502	A1	19980423	WO 1997-US18514		19971009
W: AL, AU, BA, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
CA 2268098	AA	19980423	CA 1997-2268098		19971009
AU 9749023	A1	19980511	AU 1997-49023		19971009
AU 738341	B2	20010913			
EP 932598	A1	19990804	EP 1997-911715		19971009
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
BR 9712530	A	19991019	BR 1997-12530		19971009
JP 2001506974	T2	20010529	JP 1998-518519		19971009
NO 9901677	A	19990609	NO 1999-1677		19990409
KR 2000049048	A	20000725	KR 1999-703117		19990410
PRIORITY APPLN. INFO.:			US 1996-28322P	P	19961011
			WO 1997-US18514	W	19971009

OTHER SOURCE(S): MARPAT 128:321926

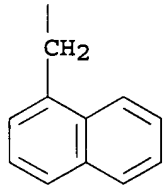
IT **206863-61-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aspartate ester inhibitors of interleukin-1β converting enzyme)

RN 206863-61-8 HCAPLUS
CN 1-Naphthaleneacetic acid, 4-carboxy-3-[[2-methyl-1,3-dioxo-3-(2-thienyl)propyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



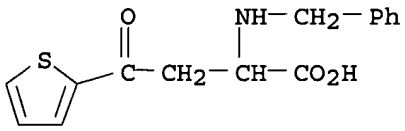
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 16 Apr 1998
AB β-Thienoylacrylic acid was prepared and then allowed to react with hydrazines, semicarbazide, thiosemicarbazide, primary amines, hydroxylamine, hydrochloride, cyanoacetamide, aromatic hydrocarbons, and/or hydrogen peroxide. Some of the obtained compds. showed interesting antibacterial and antifungal activities in vitro.
ACCESSION NUMBER: 1998:213733 HCAPLUS
DOCUMENT NUMBER: 128:243902
TITLE: Some cyclization reactions with β-thienoylacrylic acid as possible antimicrobial agents
AUTHOR(S): Salman, Asmaa Said Salem
CORPORATE SOURCE: Chemistry Department, Faculty of Science, Girls Branch, Al-Azhar University, Nasr, Egypt
SOURCE: Al-Azhar Bulletin of Science (1996), 7(2), 1179-1189
CODEN: ABSCE7; ISSN: 1110-2535

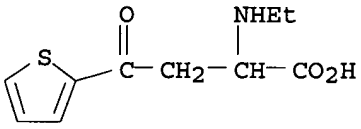
Young, Shawquia

30/05/2006

PUBLISHER: Al-Azhar University, Faculty of Science
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **204910-46-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antibacterial and antifungal activities of thienoylacrylic acid derivs.)
RN 204910-46-3 HCAPLUS
CN 2-Thiophenebutanoic acid, γ-oxo-α-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



IT **204910-36-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antibacterial and antifungal activities of thienoylacrylic acid derivs.)
RN 204910-36-1 HCAPLUS
CN 2-Thiophenebutanoic acid, α-(ethylamino)-γ-oxo- (9CI) (CA INDEX NAME)



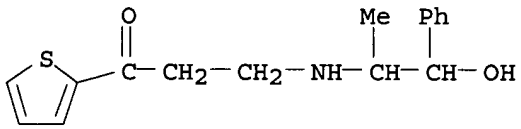
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 27 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 17 Aug 1996
AB Thiofedrine inhibited rat platelet aggregation and intraplatelet thromboxane B2 (TxB2) generation induced by arachidonic acid. The IC50 values were 0.18 and 0.21 mmol/l, resp. Thiofedrine, 1.25-5.00 mg/kg i.v., showed a significant inhibition of rat platelet aggregation and intraplatelet TxB2 generation induced by arachidonic acid, with ID50 values of 2.4 and 3.3 mg/kg. Thiofedrine, 0.5-2.0 mg/kg i.v., reduced TxB2 generation but increased 6-keto-PGF1α formation in rat plasma.
ACCESSION NUMBER: 1996:491939 HCAPLUS
DOCUMENT NUMBER: 125:212183
TITLE: Effects of thiofedrine on platelet aggregation, thromboxane B2 and 6-keto-PGF1α in rats
AUTHOR(S): Qu, Yun-Zhi; Wang, Yue-E.; Li, Xi-Xian
CORPORATE SOURCE: Department Pharmacology, Inner Mongolia Medical College, Huhhot, Peop. Rep. China
SOURCE: Methods and Findings in Experimental and Clinical Pharmacology (1996), 18(5), 297-300
CODEN: MFEPDX; ISSN: 0379-0355
PUBLISHER: Prous
DOCUMENT TYPE: Journal

Young, Shawquia

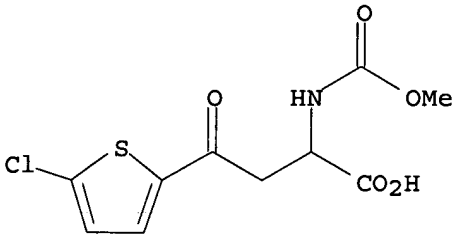
30/05/2006

LANGUAGE: English
IT **28745-69-9**, 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-hydrochloride
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(effects of thiofedrine on platelet aggregation, thromboxane B2 and 6-keto-PGF1α in rats)
RN 28745-69-9 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)

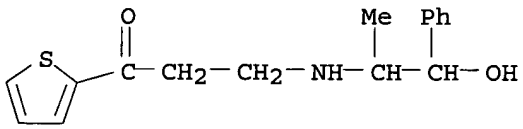


● HCl

L4 ANSWER 28 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 16 Feb 1995
AB N-protected 2-aminobutanoic acids RCH2CH2CH(NHCO2Me)CO2H (R = p-ClC6H4, Ph, p-anisyl, 5-chloro-2-thienyl, 2,5-dichloro-3-thienyl) were prepared in good yields by reduction of ketones RCOCH2CH(NHCO2Me)CO2H with Et3SiH in the presence of TiCl4. The reduction proceeded without racemization and was successfully applied to the synthesis of (R)- and (S)-p-ClC6H4CH2CH2CH(NH2)CO2H.
ACCESSION NUMBER: 1995:357581 HCAPLUS
DOCUMENT NUMBER: 123:143273
TITLE: Reduction of aromatic ketones into methylenes using triethylsilane and titanium tetrachloride. Synthesis of 2-aminobutanoic acids
AUTHOR(S): Yato, Michihisa; Homma, Koichi; Ishida, Akihiko
CORPORATE SOURCE: Org. Chem. Res. Lab., Tanabe Seiyaku Co., Ltd., Saitama, 335, Japan
SOURCE: Heterocycles (1995), 41(1), 17-20
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:143273
IT **166764-45-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of aryl-substituted aminobutanoic acids by reduction of oxo derivs. with triethylsilane and titanium tetrachloride)
RN 166764-45-0 HCAPLUS
CN 2-Thiophenebutanoic acid, 5-chloro-α-[(methoxycarbonyl)amino]-γ-oxo- (9CI) (CA INDEX NAME)



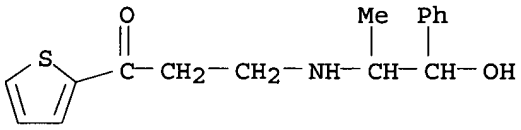
L4 ANSWER 29 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 24 Dec 1994
AB Platelet aggregation and cAMP production were studied by turbidimetry and competitive protein binding assay, resp., in rats. Thiofedrine (Thi) significantly inhibited ADP-induced and thrombin-induced platelet aggregation in vitro, with IC50 values of 0.56 and 0.16 mmol/L, resp. In vivo, Thi 1.25-5.0 mg/kg i.v. significantly inhibited ADP-induced platelet aggregation at rate of 17.1-40.3%. Thi caused a dose-dependent increase in cAMP levels in rat washed platelets. Malondialdehyde (MDA) levels in rat platelets were measured by colormetry. Thi had an inhibitory effect on thrombin-induced platelet MDA production The results suggest that the antiaggregatory action of Thi may be related to metabolism of arachidonic acid (AA) and elevation of cAMP levels.
ACCESSION NUMBER: 1994:692291 HCAPLUS
DOCUMENT NUMBER: 121:292291
TITLE: Influence of thiofedrine on platelet aggregation, intraplatelet cyclic AMP and malondialdehyde in rats
AUTHOR(S): Qu, Yun-Zhi; Li, Xi-Xian
CORPORATE SOURCE: Dep. Pharmacol., Inner Mongolia Medical College, Huhehot, Peop. Rep. China
SOURCE: Methods and Findings in Experimental and Clinical Pharmacology (1994), 16(4), 253-6
CODEN: MFEPDX; ISSN: 0379-0355
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **28745-68-8**
RL: BIOL (Biological study)
(platelet aggregation inhibitor)
RN 28745-68-8 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-(9CI) (CA INDEX NAME)



L4 ANSWER 30 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 26 Nov 1994
AB Thiofedrine inhibited platelet aggregation and thrombosis in vitro and in vivo in rats. Thiofedrine may be useful for treatment of coronary heart disease.
ACCESSION NUMBER: 1994:645672 HCAPLUS

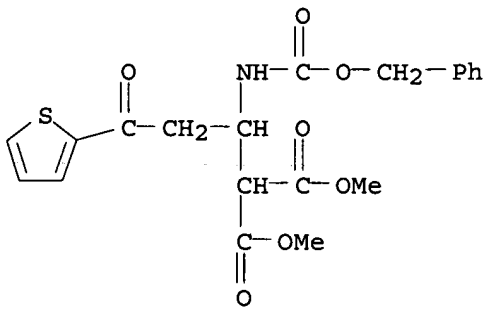
30/05/2006

DOCUMENT NUMBER: 121:245672
TITLE: Effects of thiofedrine on thrombosis in rats
AUTHOR(S): Qu, Yunzhi; Li, Daping; Pan, Jie; Li, Xixian; Zhang, Wenxing
CORPORATE SOURCE: Dep. Pharmacology, Innex Mongolia Med. Coll., Huhhot, 010059, Peop. Rep. China
SOURCE: Zhongguo Yiyao Gongye Zazhi (1994), 25(4), 170-2
CODEN: ZYGZEA; ISSN: 1001-8255
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
IT **28745-68-8**, Thiofedrine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thiofedrine inhibition of thrombosis in coronary heart disease)
RN 28745-68-8 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)- (9CI) (CA INDEX NAME)

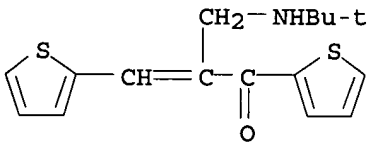


L4 ANSWER 31 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 05 Oct 1991
AB Alkylation of benzyl vinylcarbamate (I) and propene with the anions of di-Et methylmalonate or di-Me malonate in the presence of palladium(II) chloride, followed by cross-coupling or carbonylative cross-coupling with organostannanes, effected an overall dialkylation or alkylation/acylation of the monoolefin substrate. Thus, a solution of I and PdCl2(MeCN)2 in THF was treated with NaCMe(CO2Et)2 at -78° and then CH2:CHSnMe3 at -30° and the solution warmed to room temperature to give 80% (EtO2C)2CMeCH(CH2CH:CH2)NHCO2CH2Ph. Complete control of stereochem. in this palladium(II)-assisted reaction was observed by using optically active ene carbamates, affording β-amino unsatd. keto esters in good chemical yields and excellent optical purity.
ACCESSION NUMBER: 1991:535148 HCAPLUS
DOCUMENT NUMBER: 115:135148
TITLE: Palladium(II)-assisted dialkylation and alkylation/acylation of optically active ene carbamates via trialkylorganostannane cross-coupling and carbonylative coupling processes
AUTHOR(S): Masters, John J.; Hegedus, Louis S.; Tamariz, Joaquin
CORPORATE SOURCE: Dep. Chem., Colorado State Univ., Fort Collins, CO, 80523, USA
SOURCE: Journal of Organic Chemistry (1991), 56(19), 5666-71
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:135148
IT **135741-08-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 135741-08-1 HCAPLUS
CN Propanedioic acid, [3-oxo-1-[[(phenylmethoxy)carbonyl]amino]-3-(2-

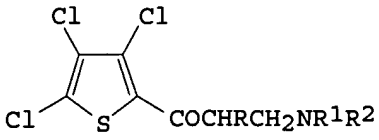
thienyl)propyl]-, dimethyl ester (9CI) (CA INDEX NAME)



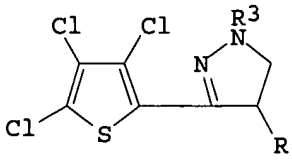
L4 ANSWER 32 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 24 Feb 1985
AB Keto-allylic systems with a heterocyclic ring in γ-position, i.e. RCH:CH(CH2Br)COR1 (R = 2-furyl, R1 = Ph; R = 2-thienyl, R1 = Ph, 2-thienyl, OMe), were prepared These undergo nucleophilic substitution reactions with amines, in which replacement of Br at the bromomethyl group takes place in contrast to the benzene analogs, where the nucleophile attacks the γ-C of the keto-allylic system.
ACCESSION NUMBER: 1985:62010 HCAPLUS
DOCUMENT NUMBER: 102:62010
TITLE: Nucleophilic substitution reaction of keto-allylic systems with a heterocyclic ring in γ-position
AUTHOR(S): Zvak, Vladimir; Kovac, Jaroslav; Dandarova, Miloslava; Gracza, Tibor; Kriz, Miroslav
CORPORATE SOURCE: Dep. Org. Chem., Slov. Inst. Technol., Bratislava, 812 37, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1984), 49(8), 1764-73
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:62010
IT **93698-46-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 93698-46-5 HCAPLUS
CN 2-Propen-1-one, 2-[[(1,1-dimethylethyl)amino]methyl]-1,3-di-2-thienyl- (9CI) (CA INDEX NAME)



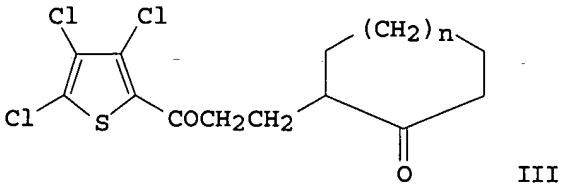
L4 ANSWER 33 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 29 Sep 1984
GI



I



II



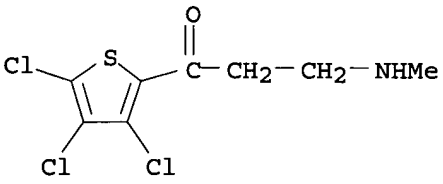
III

AB Mannich bases I [R = H, Me, R1 = R2 = Me, R1 = H, R2 = Me, Et, PhCH2; R1R2 = (CH2)5, (CH2)4O] were prepared and then they were treated with H2NNHR3 (R3 = H, Ph) to give the corresponding hydrazones, which were cyclized to give 50.5-84.6% pyrazoles II (R = H, Me; R3 = H, Ph). Treating I (R = H, R1 = R2 = Me) with cyclohexanone and cyclopentanone gave III (n = 0, 1).

ACCESSION NUMBER: 1984:510812 HCAPLUS
DOCUMENT NUMBER: 101:110812
TITLE: Studies on the chlorination of organic compounds and transformations of chlorinated derivatives. XIX. Aminomethylation of 2-acyl-3,4,5-trichlorothiophenes and the study of some reactions of Mannich bases
AUTHOR(S): Saakyan, A. M.; Safaryan, A. A.; Akopyan, A. N.
CORPORATE SOURCE: USSR
SOURCE: Armyanskii Khimicheskii Zhurnal (1984), 37(4), 261-5
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 101:110812

IT **91707-96-9P 91707-97-0P 91707-98-1P 91708-00-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

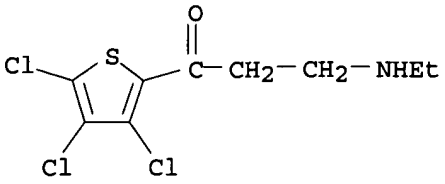
RN 91707-96-9 HCAPLUS
CN 1-Propanone, 3-(methylamino)-1-(3,4,5-trichloro-2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

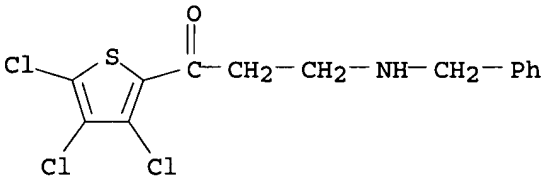
RN 91707-97-0 HCAPLUS
CN 1-Propanone, 3-(ethylamino)-1-(3,4,5-trichloro-2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)

Young, Shawquia



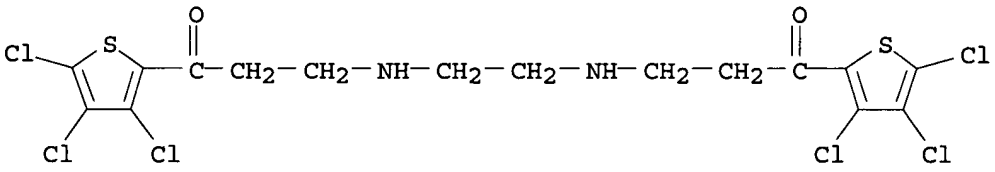
● HCl

RN 91707-98-1 HCAPLUS
CN 1-Propanone, 3-[(phenylmethyl)amino]-1-(3,4,5-trichloro-2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



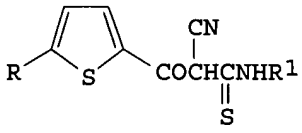
● HCl

RN 91708-00-8 HCAPLUS
CN 1-Propanone, 3,3'-(1,2-ethanediyldiimino)bis[1-(3,4,5-trichloro-2-thienyl)-, dihydrochloride (9CI) (CA INDEX NAME)

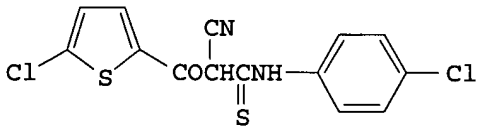


●2 HCl

L4 ANSWER 34 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
GI



I



II

AB Title compds. (I; R = H, halo, lower alkyl or alkoxy; R1 = C3-6 cycloalkyl, aryl, furfuryl) and their salts were prepared as inflammation inhibitors (no data). Thus, 2-(bromoacetyl)-5-chlorothiophene was treated with KCN and the product nitrile treated with 4-ClC6H4NCS to give the title compound II.

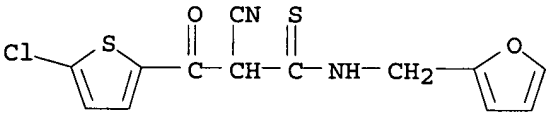
ACCESSION NUMBER: 1984:68161 HCAPLUS
DOCUMENT NUMBER: 100:68161
TITLE: Substituted thenoylthiocarbamoylacetonitriles and pharmaceutical preparations containing them
INVENTOR(S): Uhlendorf, Joachim; Leyck, Sigurd
PATENT ASSIGNEE(S): Nattermann, A., und Cie. G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 11 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3217446	A1	19831124	DE 1982-3217446	19820508

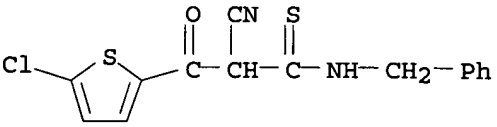
PRIORITY APPLN. INFO.: DE 1982-3217446 19820508
OTHER SOURCE(S): CASREACT 100:68161; MARPAT 100:68161

IT **88579-07-1P 88579-13-9P 88579-15-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as inflammation inhibitor)

RN 88579-07-1 HCAPLUS
CN 2-Thiophenepropanethioamide, 5-chloro-α-cyano-N-(2-furanylmethyl)-β-oxo- (9CI) (CA INDEX NAME)

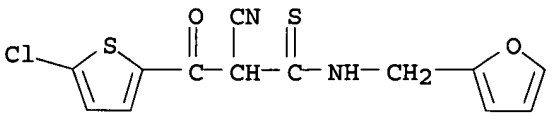


RN 88579-13-9 HCAPLUS
CN 2-Thiophenepropanethioamide, 5-chloro-α-cyano-β-oxo-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

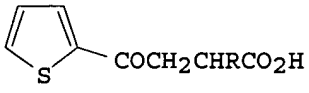


RN 88579-15-1 HCAPLUS
CN 2-Thiophenepropanethioamide, 5-chloro-α-cyano-N-(2-furanylmethyl)-

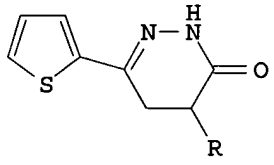
β-oxo-, sodium salt (9CI) (CA INDEX NAME)



L4 ANSWER 35 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
GI



II

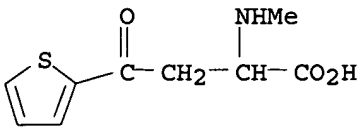


III

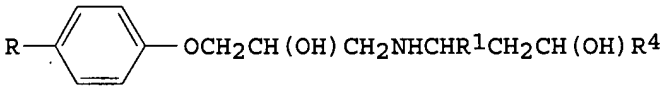
AB Treatment of 3-(thenoyl)acrylic acid (I) with indole, 2-methylindole, and Et 2-methylpyrrole-3-carboxylate gave 64-93% II [R = indol-3-yl, 2-methylindol-3-yl, 2-methyl-3-(ethoxycarbonyl)pyrrol-5-yl] and 70-97% of the corresponding Me esters. Cyclization of II by N2H4.H2O gave 63-96% III (R as above). Amination of I with NH3 gave 75% amide. Addnl. obtained were 67-86% amides from MeNH2, piperidine, morpholine, aziridine and imidazole.

ACCESSION NUMBER: 1981:156662 HCAPLUS
DOCUMENT NUMBER: 94:156662
TITLE: Reaction of β-thenoylacrylic acid with some nucleophilic reagents
AUTHOR(S): Grigoryan, G. V.; Agbalyan, S. G.
CORPORATE SOURCE: Inst. Org. Khim., Yerevan, USSR
SOURCE: Armyanskii Khimicheskii Zhurnal (1980), 33(10), 856-61
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 94:156662

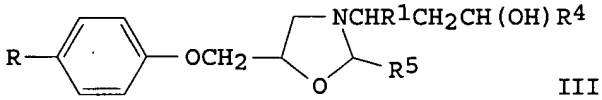
IT **77253-25-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 77253-25-9 HCAPLUS
CN 2-Thiophenebutanoic acid, α-(methylamino)-γ-oxo- (9CI) (CA INDEX NAME)



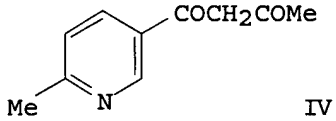
L4 ANSWER 36 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
GI



I



III



IV

AB A process was claimed for the preparation of the title compds. I [R = alkoxymethyl, alkoxyalkoxy, hydroxyalkoxy, NHCONR2R3 (R2 and R3 = H, alkyl, alkenyl, cycloalkyl; NR2R3 = a saturated 5- or 6-membered monocyclic heterocyclic group, if necessary, having an O or S as addnl. hetero atom, and containing C1-4 alkyl or alkoxy, C3-4 alkenyl, C5-7 cycloalkyl groups); R1 = H, Me; R4 = a C-bound aromatic or quasi-aromatic 5- or 6-membered monocyclic ring with 1 or 2 N, O, and(or) S atoms, which can be substituted by 1 or more Me groups] as well as their aldehyde condensation products and acid addition salts, whereby one hydrogenates 4-RC6H4OCH2CH(OH)CH2NHCR1:CHCOR4 (II), 4-RC6H4OCH2COCH2NHCR1:CHCOR4, or 4-RC6H4OCH2COCH2NHCHR1CH2CH(OH)R4, or, if one preps. I (R1 = H), one hydrogenates 4-RC6H4OCH2COCH2NHCH2CH2COR4 or 4-RC6H4OCH2CH(OH)CH2NHCH2CH2COR4 and one converts the compound formed into an oxazolidine III (R5 = H, C1-4 alkyl) with R5CHO, or, if necessary, with an acid into an acid addition salt. Thus, 4-MeO(CH2)4OC6H4OCH2CH(OH)CH2NH2, nicotinoylacetone IV, EtOH, and HCO2H were heated to 50° and stirred an addnl. 20 h at room temperature to give II [R = MeO(CH2)4O, R1 = Me, R4 = 2-methyl-5-pyridyl] which was reduced with NaBH4 at 70° in EtOH 7 h to give the corresponding I. IV was prepared by stirring 5-acetyl-α-picoline, PhMe, EtOAc, and KOCMe3 20 h at 40°. An addnl. 27 I, 2 I salts, and 1 III were prepared Selected I had ED50 0.003-0.093 mg/kg (dog), as β1-receptor inhibitors and ED50 1.02-15.59 mg/kg (dog) as β2-receptor inhibitors [vs. 0.238 and 26.505 for 4-Me2CHNHCH2CH(OH)CH2OC6H4NHAc] and are useful in treating arrhythmia and other heart disorders.

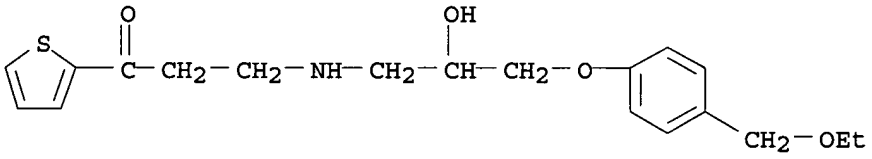
ACCESSION NUMBER: 1978:105151 HCAPLUS
DOCUMENT NUMBER: 88:105151
TITLE: 1-Phenoxy-3-aminopropan-2-ol derivatives and their acid addition salts
PATENT ASSIGNEE(S): Cassella Farbwerke Mainkur A.-G., Fed. Rep. Ger.
SOURCE: Austrian, 14 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

Young, Shawquia

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 339305	B	19771010	AT 1974-10164	19741219
AT 7410164	A	19770215		
US 4088764	A	19780509	US 1974-531344	19741210
FI 7403631	A	19750628	FI 1974-3631	19741216
NO 7404530	A	19750630	NO 1974-4530	19741216
SE 7415761	A	19750630	SE 1974-15761	19741216
DK 7406547	A	19750825	DK 1974-6547	19741216
DD 117071	C	19751220	DD 1974-183198	19741219
ZA 7408082	A	19760128	ZA 1974-8082	19741219
SU 559643	D	19770525	SU 1974-2085461	19741219
SU 598557	D	19780315	SU 1974-2085234	19741219
HU 171726	P	19780328	HU 1974-CA376	19741219
CA 1047512	A1	19790130	CA 1974-216421	19741219
US 4066768	A	19780103	US 1976-669995	19760324

PRIORITY APPLN. INFO.: LU 1973-34590 A 19731227
US 1974-531344 A2 19741210

IT **65752-91-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
RN 65752-91-2 HCAPLUS
CN 1-Propanone, 3-[[3-[4-(ethoxymethyl)phenoxy]-2-hydroxypropyl]amino]-1-(2-thienyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 37 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB Thirty-two RCOCH2CH2NHCHMeCHPhOH (I, R = heterocyclyl), useful for treatment of heart disease at 0.1-500 mg oral doses, were prepared by treating l-norephedrine with acetyl derivative of the appropriate heterocycle. Thus, a mixture of 12.6 g 2-acetylthiophene, 18.7 g l-norephedrine hydrochloride, 4 g paraformaldehyde in 20 ml Me2CHOH was refluxed with 0.2 mole concentrated HCl for 2 hr to give 17 g I (R = 2-thienyl).

ACCESSION NUMBER:	1975:443189 HCAPLUS
DOCUMENT NUMBER:	83:43189
TITLE:	Indole aminoketones
INVENTOR(S):	Posselt, Klaus; Thiele, Kurt
PATENT ASSIGNEE(S):	Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler, Fed. Rep. Ger.
SOURCE:	U.S., 8 pp. Continuation-in-part of U. S. 3,658,845 (CA 77;19630s). CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	5

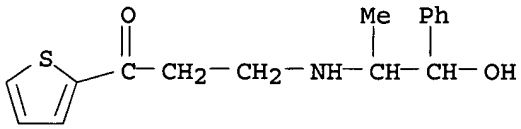
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 3859305	A	19750107	US 1971-137575		19710426
US 3514465	A	19700526	US 1967-693138		19671226
US 3658845	A	19720425	US 1970-18300		19700310
PRIORITY APPLN. INFO.:			US 1967-693138	A3	19671226
			US 1970-18300	A2	19700310
			DE 1966-D51910	A	19661230
			DE 1966-D51911	A	19661230

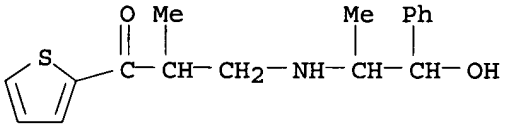
IT **28745-69-9P 28745-89-3P 28745-90-6P**
28763-18-0P 38977-57-0P 55895-74-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 28745-69-9 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



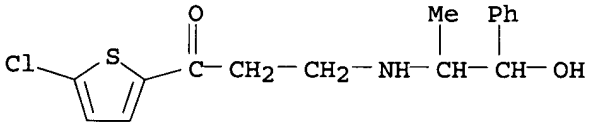
● HCl

RN 28745-89-3 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-2-methyl-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

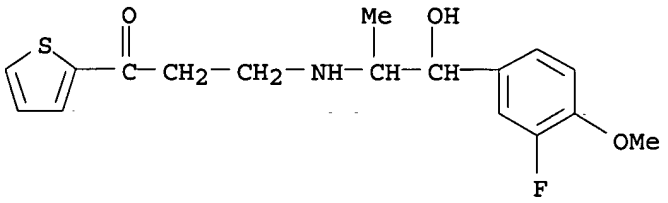
RN 28745-90-6 HCAPLUS
CN 1-Propanone, 1-(5-chloro-2-thienyl)-3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

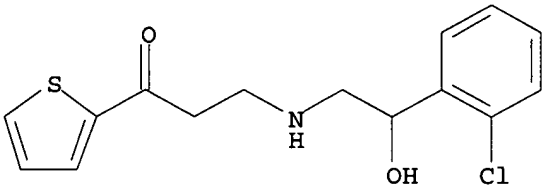
RN 28763-18-0 HCAPLUS

CN 1-Propanone, 3-[[2-(3-fluoro-4-methoxyphenyl)-2-hydroxy-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride, (+)- (9CI) (CA INDEX NAME)



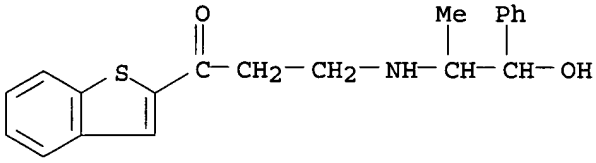
● HCl

RN 38977-57-0 HCAPLUS
CN 1-Propanone, 3-[[2-(2-chlorophenyl)-2-hydroxyethyl]amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 55895-74-4 HCAPLUS
CN 1-Propanone, 1-benzo[b]thien-2-yl-3-[(2-hydroxy-1-methyl-2-phenyl)amino]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 38 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB Eight RCOCH2CH2NHCHMeCH(OH)C6H4OH-p.HCl I (R = 2-furyl, 2-, and 3-thienyl, 1-methyl-3-indolyl, etc.) were prepared Thus, 2-acetylthiophene was treated with 4-hydroxynorephedrine.HCl and paraformaldehyde to give I (R = 2-thienyl). At 5-500 μg I were coronary dilators. At 1.4 + 10-5

Young, Shawquia

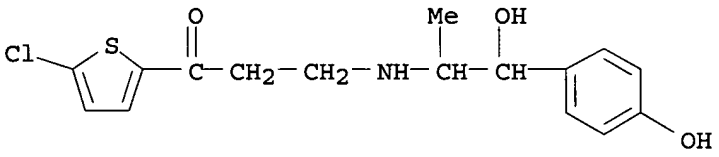
to 2.8 + 10-7 g/ml I had bronchospasmolytic activity. I were antiphlogistic at 10-500 mg/kg.

ACCESSION NUMBER: 1974:413378 HCAPLUS
DOCUMENT NUMBER: 81:13378
TITLE: 3-(3-[1-(4-Hydroxyphenyl)-1-hydroxypropyl-(2)-amino]-propionyl-thiophene
INVENTOR(S): Posselt, Klaus
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3803173	A	19740409	US 1971-137576	19710426
PRIORITY APPLN. INFO.:			US 1971-137576 A	19710426

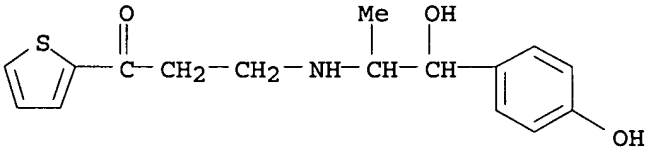
IT **35056-53-2P 35056-56-5P 35056-57-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35056-53-2 HCAPLUS
CN 1-Propanone, 1-(5-chloro-2-thienyl)-3-[[2-hydroxy-2-(4-hydroxyphenyl)-1-methylethyl]amino]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

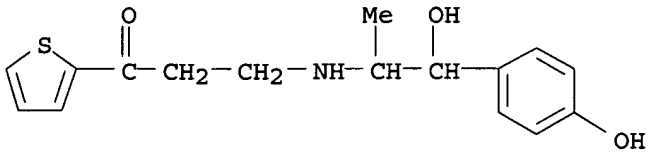
RN 35056-56-5 HCAPLUS
CN 1-Propanone, 3-[[2-hydroxy-2-(4-hydroxyphenyl)-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 35056-57-6 HCAPLUS
CN 1-Propanone, 3-[[2-hydroxy-2-(4-hydroxyphenyl)-1-methylethyl]amino]-1-(2-thienyl)- (9CI) (CA INDEX NAME)

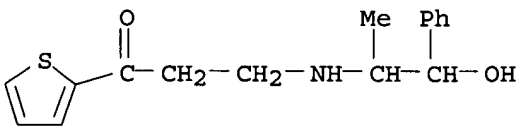
Young, Shawquia



L4 ANSWER 39 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB The ketone (I, R = α-thienyl, α-furyl, 3-pyridyl, 2,4-dimethyl-5-thiazolyl, 3-benzothiophenyl, 3-quinolyl, etc. R1 = H, OMe, R2 = H, F; R3 = H,Cl) were prepared by treating an acetylheterocycle with norephedrine or its derivs. and paraformaldehyde. Thus, 12.6 g 2-acetylthiophene was treated with 18.7 g 1-norephedrine-HCl and 4 g paraformaldehyde to give 17 g I(R = 2-thienyl R1 = R2 = R3 = H). Several I were reduced to the corresponding alcs. I increased the cerebral and peripheral blood flow in narcotized dogs.
ACCESSION NUMBER: 1973:136051 HCAPLUS
DOCUMENT NUMBER: 78:136051
TITLE: 2-3-Phenyl-3(hydroxypropylamino) ethyl-3-thienyl ketone
INVENTOR(S): Posselt, Klaus; Thiele, Kurt
SOURCE: U.S., 7 pp. Continuation-in-part of U.S. 3,514,465 (CA 73;7724n).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

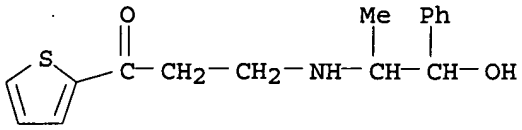
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 3715369	A	19730206	US 1970-23455		19700327
DE 1670547	A	19701112	DE 1966-D51911		19661230
DE 1543538	A1	19760205	DE 1966-D51910		19661230
US 3514465	A	19700526	US 1967-693138		19671226
PRIORITY APPLN. INFO.:			DE 1966-D51911	A	19661230
			US 1967-693138	A	19671226
			DE 1966-D51910		19661230

IT **28745-68-8P 28745-69-9P 28745-89-3P**
28745-90-6P 28763-18-0P 38977-57-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-68-8 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)- (9CI) (CA INDEX NAME)



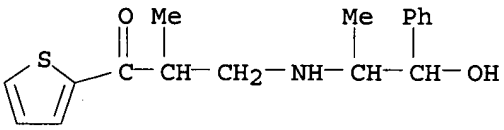
RN 28745-69-9 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-,

hydrochloride (9CI) (CA INDEX NAME)



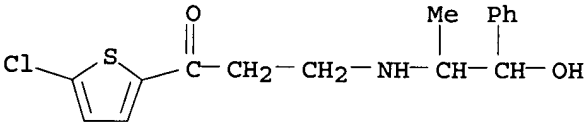
● HCl

RN 28745-89-3 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-2-methyl-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



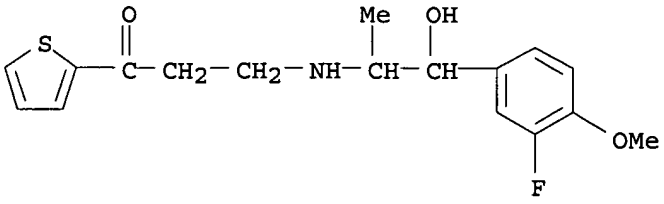
● HCl

RN 28745-90-6 HCAPLUS
CN 1-Propanone, 1-(5-chloro-2-thienyl)-3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-, hydrochloride (9CI) (CA INDEX NAME)



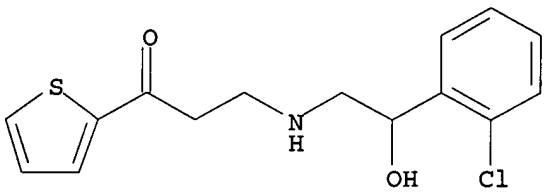
● HCl

RN 28763-18-0 HCAPLUS
CN 1-Propanone, 3-[[2-(3-fluoro-4-methoxyphenyl)-2-hydroxy-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride, (+)- (9CI) (CA INDEX NAME)



● HCl

RN 38977-57-0 HCAPLUS
CN 1-Propanone, 3-[[2-(2-chlorophenyl)-2-hydroxyethyl]amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 40 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB About 30 aminoketones RCOCHR1CH2NHCH2CH(OH)C6H4R2 (I, R = 1,3,5-trimethyl-4-pyrazolyl, 2,4-dimethylthiazolyl, 1,3-dimethyl-4-pyrazolyl, 1-benzyl-2,4-pyrazolyl, thienyl, methylenedioxyphenyl etc., R1 = H, Me, R2 = H, Cl, 3,4-Cl(MeO)) were prepared from 1-norephedrine-hCl and acetyl heterocycles. Thus, 27 g 1,2,3-trimethylacetyl-pyrazole was treated with 33 g 1-norephedrine-HCl, paraformaldehyde, and concentrated HCl to give 14.5 g I (R = 1,3,5-trimethyl-4-pyrazolyl).

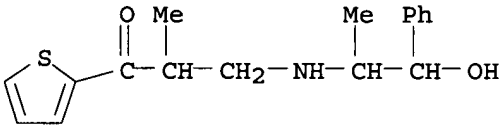
ACCESSION NUMBER: 1972:552179 HCAPLUS
DOCUMENT NUMBER: 77:152179
TITLE: Pyrazole and pyrazolinone amino ketones
INVENTOR(S): Posselt, Klaus; Enkheim, Bergen; Thiele, Kurt
PATENT ASSIGNEE(S): deut ge
SOURCE: U.S., 6 pp. Continuation-in-part of U.S. 3,514,465 (CA 76;72214n).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3686206	A	19720822	US 1970-19511	19700313
DE 1670547	A	19701112	DE 1966-D51911	19661230
DE 1543538	A1	19760205	DE 1966-D51910	19661230

FR 8021	M	19700803	FR 1967-8021		19671229
GB 1203810	A	19700903	GB 1967-1203810		19671229
AT 286978	B	19710111	AT 1967-11809		19671229
PRIORITY APPLN. INFO.:			DE 1966-D51910	A	19661230
			DE 1966-D51911	A	19661230

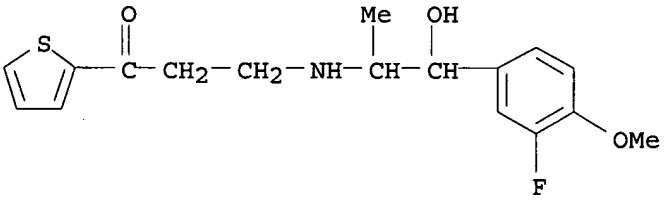
IT **28745-89-3P 28763-18-0P 35576-10-4P**
35580-28-0P 38977-57-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 28745-89-3 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-2-methyl-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

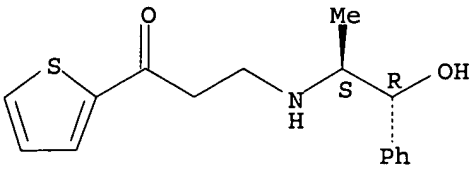
RN 28763-18-0 HCAPLUS
CN 1-Propanone, 3-[[2-(3-fluoro-4-methoxyphenyl)-2-hydroxy-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride, (+)- (9CI) (CA INDEX NAME)



● HCl

RN 35576-10-4 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-, hydrochloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

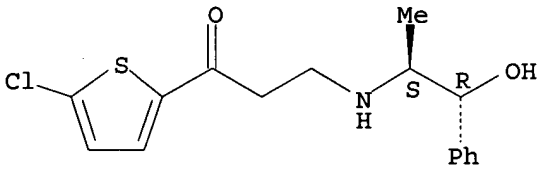
Absolute stereochemistry.



● HCl

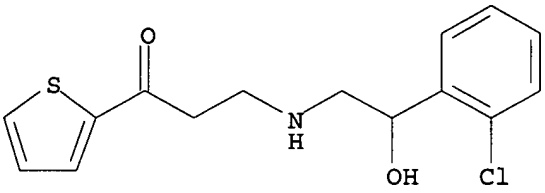
RN 35580-28-0 HCAPLUS
CN 1-Propanone, 1-(5-chloro-2-thienyl)-3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-, hydrochloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

RN 38977-57-0 HCAPLUS
CN 1-Propanone, 3-[[2-(2-chlorophenyl)-2-hydroxyethyl]amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 41 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB Division of U.S. 3,514,465 (CA73! 77214m). Twenty-four RCOCH2CH2NHCHMeCHPhOH (I,R = heterocycle) and 5 RCH(OH)CH2CH2NHCHMeCHPhOH (R = heterocycle), were prepared Thus, 4-methyl-2-acetylthiazole, norephedrine-HCl, paraformaldehyde, and HCl in iso-PrOH was refluxed 2 hr to give I.HCl (R = 4-methyl-2-thiazolyl).
ACCESSION NUMBER: 1972:419630 HCAPLUS
DOCUMENT NUMBER: 77:19630
TITLE: Benzothiophene amino ketones and amino alcohols

Young, Shawquia

30/05/2006

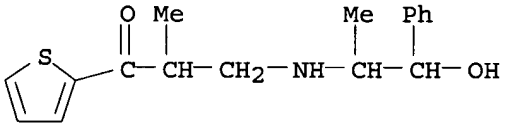
INVENTOR(S): Posselt, Klaus; Thiele, Kurt
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: U.S., 5 pp. Division of U.S. 3,514,465 (CA 73;77214m). CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3658845	A	19720425	US 1970-18300	19700310
DE 1670547	A	19701112	DE 1966-D51911	19661230
DE 1543538	A1	19760205	DE 1966-D51910	19661230
FR 8021	M	19700803	FR 1967-8021	19671229
GB 1203810	A	19700903	GB 1967-1203810	19671229
AT 286978	B	19710111	AT 1967-11809	19671229
US 3859305	A	19750107	US 1971-137575	19710426

PRIORITY APPLN. INFO.:

DE 1966-D51910	A	19661230
DE 1966-D51911	A	19661230
US 1967-693138	A3	19671226
US 1970-18300	A2	19700310

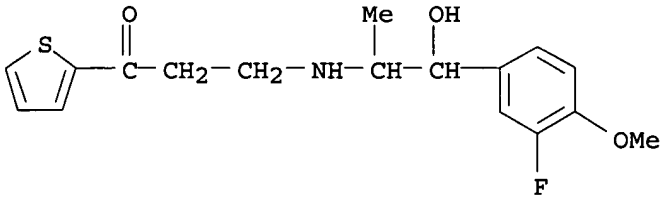
IT **28745-89-3P 28763-18-0P 35576-10-4P 35580-28-0P 37421-99-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-89-3 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-2-methyl-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 28763-18-0 HCAPLUS
CN 1-Propanone, 3-[[2-(3-fluoro-4-methoxyphenyl)-2-hydroxy-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride, (+)- (9CI) (CA INDEX NAME)

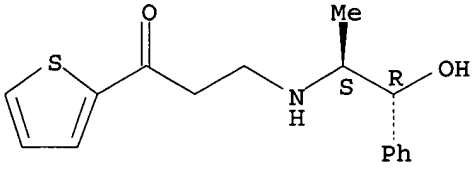
Young, Shawquia



● HCl

RN 35576-10-4 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-, hydrochloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

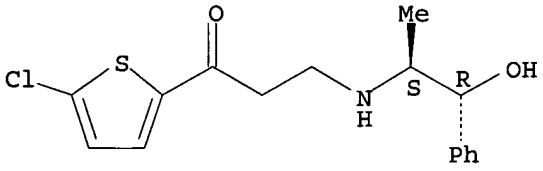
Absolute stereochemistry.



● HCl

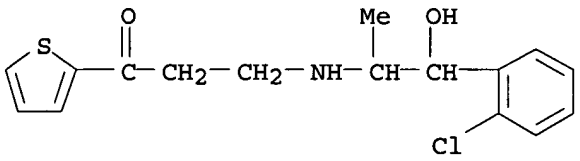
RN 35580-28-0 HCAPLUS
CN 1-Propanone, 1-(5-chloro-2-thienyl)-3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-, hydrochloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

RN 37421-99-1 HCAPLUS
CN 1-Propanone, 3-[[2-(2-chlorophenyl)-2-hydroxy-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)

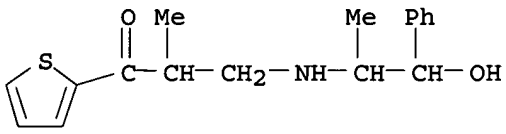


● HCl

L4 ANSWER 42 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Continuation-in-part of U.S. 3,514,465 (CA 73: 77214n). -Acetylthiophene was treated with PhCH(OH)CHMeNH2.HCl (I) and paraformaldehyde to give II (R = R1 = R2 = H) (III). About 20 analogs of III were prepared by treatment of I with paraformaldehyde and acetyl heterocycles (2-acetylfuran, acetylthiazoles, 3-acetylpyridine, acetylpyrazoles, 2-acetylbenzopyran, etc.). Two similar II (R = MeO, R1 = F, R2 = H; R = R1 = H, R2 = Cl) were prepared III and several of its analogs were reduced to the alcs. The compds. were coronary-dilating agents.
ACCESSION NUMBER: 1972:113205 HCAPLUS
DOCUMENT NUMBER: 76:113205
TITLE: Thiazolyl and pyridyl amino alcohols
INVENTOR(S): Posselt, Klaus; Thiele, Kurt
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: U.S., 6 pp. Continuation-in-part of U.S. 3,514,465 (CA 73;77214n).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3631055	A	19711228	US 1970-18279	19700310

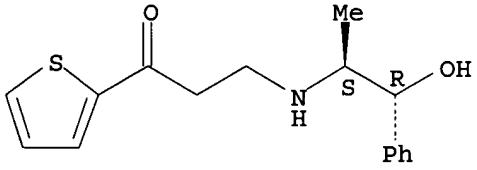
PRIORITY APPLN. INFO.: US 1970-18279 A 19700310
IT **28745-89-3P 35576-09-1P 35576-10-4P**
35580-26-8P 35580-28-0P 35580-29-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-89-3 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-2-methyl-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

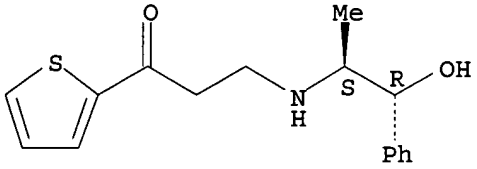
RN 35576-09-1 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 35576-10-4 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-, hydrochloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

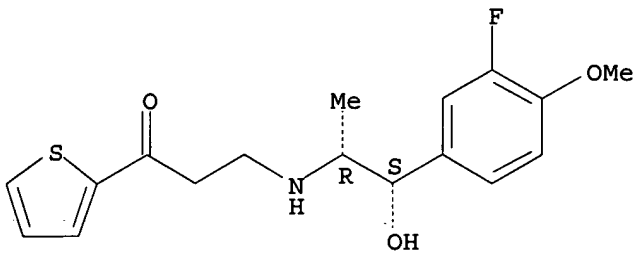
Absolute stereochemistry.



● HCl

RN 35580-26-8 HCAPLUS
CN 1-Propanone, 3-[[2-(3-fluoro-4-methoxyphenyl)-2-hydroxy-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride, (R*,S*)- (9CI) (CA INDEX NAME)

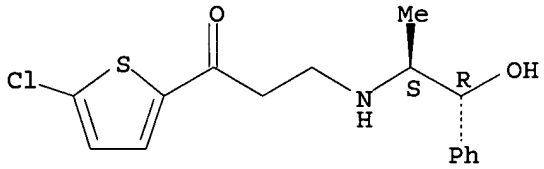
Relative stereochemistry.



● HCl

RN 35580-28-0 HCAPLUS
CN 1-Propanone, 1-(5-chloro-2-thienyl)-3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-, hydrochloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

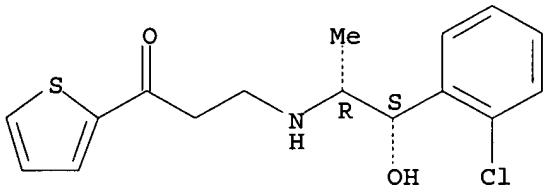
Absolute stereochemistry.



● HCl

RN 35580-29-1 HCAPLUS
CN 1-Propanone, 3-[[2-(2-chlorophenyl)-2-hydroxy-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

L4 ANSWER 43 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB Nine RCOCH2CH2NHCHMeCH(OH)C6H4OH-p.HCl (I) (e.g. R=2,5-dimethyl-3-thienyl, 2-benzofuryl, and 1-methyl-3-indolyl), papaverine-like effective on blood circulation, heart, and as bronchospasmolytic agents and salicylamide-like effective as antiinflammatory agents, were prepared by reaction of

4-hydroxynorephedrine-HCl (II) with RAc and HCHO or with RCOCH2CH2NMe2. Thus, 11 g 2-acetylfuran was refluxed 2.5 hr with 3 g paraformaldehyde and 20.5 g II in iso-PrOH to give 8 g I (R=2-furyl).

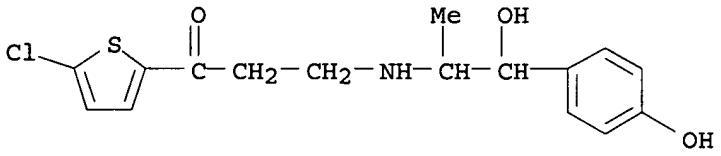
ACCESSION NUMBER: 1972:59440 HCAPLUS
DOCUMENT NUMBER: 76:59440
TITLE: 3-[2-(p-Hydroxyphenyl)-2-hydroxy-1-methylethylamino]propionyl-substituted indoles, (benzo)furans, and (benzo)thiophenes
INVENTOR(S): Posselt, Klaus
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: Ger. Offen., 23 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2121104	A	19711111	DE 1971-2121104	19710429
AT 306710	B	19730425	AT 1970-3964	19700430
CH 555333	A	19741031	CH 1971-4582	19710330
FR 2092114	A5	19720121	FR 1971-15375	19710429
FR 2092114	B1	19740823		
JP 55029978	B4	19800807	JP 1972-42562	19720426

PRIORITY APPLN. INFO.: AT 1970-3964 A 19700430

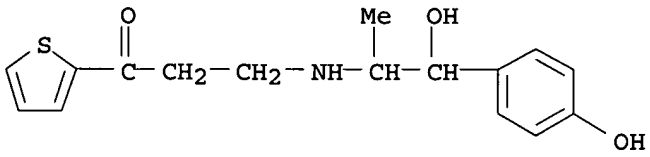
IT **35056-53-2P 35056-56-5P 35056-57-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35056-53-2 HCAPLUS
CN 1-Propanone, 1-(5-chloro-2-thienyl)-3-[[2-hydroxy-2-(4-hydroxyphenyl)-1-methylethyl]amino]-, hydrochloride (9CI) (CA INDEX NAME)



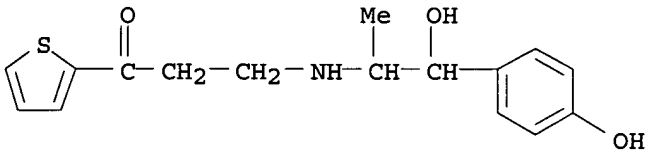
● HCl

RN 35056-56-5 HCAPLUS
CN 1-Propanone, 3-[[2-hydroxy-2-(4-hydroxyphenyl)-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 35056-57-6 HCAPLUS
CN 1-Propanone, 3-[[2-hydroxy-2-(4-hydroxyphenyl)-1-methylethyl]amino]-1-(2-thienyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 44 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB The title compds. PhCH(OH)CHMeNHC2H4COA (I), where A is a heterocyclic moiety, are stimulants to coronary blood flow. I are prepared by treating PhCH(OH)CHMeNH2 (II) with AcOMe and paraformaldehyde (III) or with AcOCH2CH2Cl or AcOCH:CH2. Thus, 12.6 g 2-acetylthiophene (IV), 18.7 g II.HCl, and 4 g III in 20 ml iso-PrOH is treated with 0.2 mole concentrated HCl and refluxed 2 hr to give the HCl salt of I (A = 2-thienyl) (V), m. 191-2°. II (1.5 g) and 2.7 g 2-thienyl vinyl ketone in 60 ml Et2O gave, after 0.5 hr, V, m. 118-20°. 2-(β-Chloropropionyl)thiophene (5.2 g), 4.5 g II, and 4 g Et3N in Me2NCHO gave V after 1 hr. Similarly, using the first method, are prepared the following I (A and m.p. HCl salt given): 2-furanyl, 186-7°; 2-(4-methylthiazolyl), 197-9°; 4-antipyryl, 206-8°; 3-pyridyl, 187-9°; 5-(2,4-dimethylthiazolyl), 208-10°; 5-(4-methyl-2-hydroxythiazolyl), 209-10°; 2-coumaronyl, 199-200°; 3-thionaphthenyl, 200-21°; 3-(1-methylindolyl), 194-5°; 3,4-methylenedioxyphenyl, 195-7°; 4-(1,3-dimethylpyrazolyl), 196°; 3-quinolyl, 205-6°; 4-isoquinolyl, 208°; 3-(1,2,4-trimethyl-5-carbethoxypyrrolyl), 178-80°; 6-(benzo-1,4-dioxanyl), 201°; 2-(benzo-1,4-dioxanyl), 178°; 4-(2-benzyl-10-hydroxydecahydroisoquinolyl), 182-3°; 2-(5-nitrofuryl), 210°; 4-(1,3,5-trimethylpyrazolyl), 191°; 4-(1-benzyl-3,5-dimethylpyrazolyl, 200°; 2-(5-chlorothienyl), 198°. Analogs of I were similarly prepared (reactants and m.p. of HCl salt of product given): (±)-[3,4-F(MeO)C6H3CH(OH)CHMeNH2].HCl, IV, III, 208°; II.HCl, 2-propionylthiophene, III, 208°; (±)-[2-ClC6H4CH(OH)CH2NH2].HCl, IV, III, 158-60°. Other active compds. are prepared by reduction of the carbonyl of I with (iso-PrO)3Al or NaBH4 to give ACH(OH)C2H4NHCHMeCH(OH)Ph (VI). Thus were prepared VI (A and m.p. of HCl salt given): 2-(4-phenylthiazolyl), 178-81°; 2-thenyl, 152-3°; 2-coumaranyl, 210-15°; 2-thionaphthenyl, 167-70°.
ACCESSION NUMBER: 1970:477214 HCAPLUS

30/05/2006

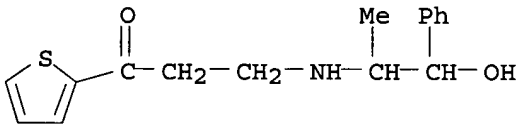
DOCUMENT NUMBER: 73:77214
TITLE: Coronary dilating 2-(3-phenyl-3-hydroxy-2-propylamino)ethyl heterocyclic ketones
INVENTOR(S): Posselt, Klaus; Enkheim, Bergen; Thiel, Kurt
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3514465	A	19700526	US 1967-693138	19671226
DE 1670547	A	19701112	DE 1966-D51911	19661230
DE 1543538	A1	19760205	DE 1966-D51910	19661230
FR 8021	M	19700803	FR 1967-8021	19671229
GB 1203810	A	19700903	GB 1967-1203810	19671229
AT 286978	B	19710111	AT 1967-11809	19671229
US 3715369	A	19730206	US 1970-23455	19700327
US 3859305	A	19750107	US 1971-137575	19710426

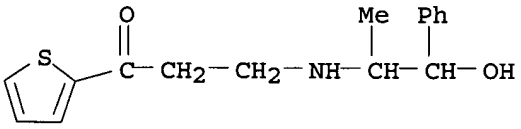
PRIORITY APPLN. INFO.:

DE 1966-D51910	A	19661230
DE 1966-D51911	A	19661230
US 1967-693138	A	19671226
US 1970-18300	A2	19700310

IT **28745-68-8P 28745-69-9P 28745-89-3P**
28745-90-6P 28763-18-0P 28763-19-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-68-8 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-(9CI) (CA INDEX NAME)



RN 28745-69-9 HCAPLUS
CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)

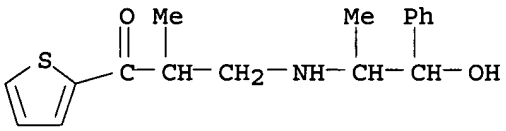


● HCl

RN 28745-89-3 HCAPLUS

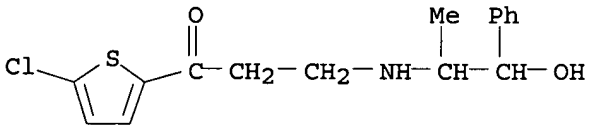
Young, Shawquia

CN 1-Propanone, 3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-2-methyl-1-(2-thienyl)-, hydrochloride (9CI) (CA INDEX NAME)



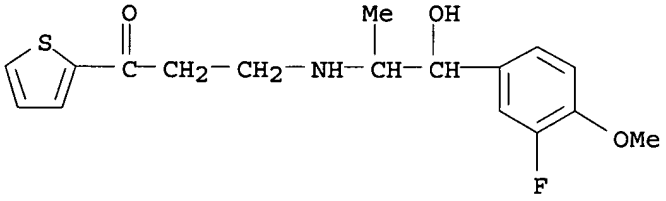
● HCl

RN 28745-90-6 HCAPLUS
CN 1-Propanone, 1-(5-chloro-2-thienyl)-3-[(2-hydroxy-1-methyl-2-phenylethyl)amino]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

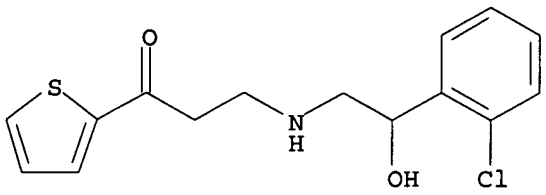
RN 28763-18-0 HCAPLUS
CN 1-Propanone, 3-[[2-(3-fluoro-4-methoxyphenyl)-2-hydroxy-1-methylethyl]amino]-1-(2-thienyl)-, hydrochloride, (+)- (9CI) (CA INDEX NAME)



● HCl

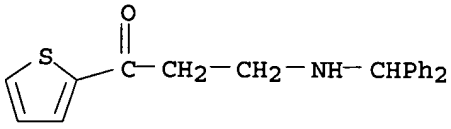
RN 28763-19-1 HCAPLUS
CN 1-Propanone, 3-[(o-chloro-β-hydroxyphenethyl)amino]-1-(2-thienyl)-, hydrochloride (8CI) (CA INDEX NAME)

Rotation (+).



● HCl

L4 ANSWER 45 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB Aralkyl amines Ph2CH(CH2)xNH(CH2)yPh.-HCI (I), Ph2CHNHCHMe(CH2)xPh.HCl (II), Ph2CHNHCH2CH2CO R (III), and RR1NCHPhCH2COR2 (IV) are prepared Thus, 1 mole organic chlorides Ph2CH(CH2)xCl are treated with 1-4 moles amines H2N(CH2)yPh to give 57% N-(3,3-diphenylpropyl)-N-(phenethyl)amine-HCl, m. 207°, and the following I (x, y, m.p., and % yield given): 2, 1, 179°, 36; 2, 0, 215°, 16; 1, 1, 260°, 31; 0, 1, 238°, 34. Similarly prepared, from Ph2CHBr, are (m.p. and % yield given): II (x = 1), 203-9°, 32; II (x = 0), 245°, 52. Benzhydrylamine (0.01 mole) is treated with 0.01 mole amino ketone RCOCH2CH2NMe2.HCl to give 38% N-benzhydryl-N-(2-benzoylethyl)amine, m. 110°, and the following III (R. m.p., and % yield given): p-HOC6H4, 148°, 55; p-MeOC6H4, 105°, 40: p-CiC6H4, 118°, 50; p-BrC6H4, 118°, 50; 2-C10H7, 120°,30: 2-thienyl, 56°, 56. Ketones PhCH:-CHCOR2 (0.01 mole) are heated with amines RR1NH to give the following IV [RR1N, R2, and m.p. given]: piperidino, tert-Bu, 65-6°; morpholino, tert-Bu, 87°; NHPh, tert-Bu, 153°; p-Me2NC6H4NH, Ph, 160°. Also prepared (according to related and known methods) are the following related compds. (m.p. given): Ph2CHCH2CONHCHMeCH2Ph, 180-10°; Ph2CHNHCH2NHCHPh2, 232°; Ph2CHNHCH2CH2C(:NOH)Ph, 125°; Ph2CHNHCH2CH2CHPhNH2-2HCl,255°; Ph2NCH2CH2-C(:NOH)Ph, 130°; Ph2NCH2CH2CHPhNH2.HCl, 214°; Ph2CHNHCH2COPh, 125°; 1,1 - diphenyl - 4 - (3 - methylpiperidino)-2-butanone-HCl, 194°; MeCH(NO2)CH2NHCH2CH2Ph.-HCl, 125°; MeCH(NO2)CH2NHCH2Pr-iso.-HCl, 180°.
ACCESSION NUMBER: 1969:501431 HCAPLUS
DOCUMENT NUMBER: 71:101431
TITLE: Analogs of prenylamine [as potential coronary vasodilators]
AUTHOR(S): Collino, Franco
CORPORATE SOURCE: Inst. Chem. Farm. Tossicol., Univ. Trieste, Trieste, Italy
SOURCE: Bollettino Chimico Farmaceutico (1969), 108(6), 255-67
CODEN: BCFAAI; ISSN: 0006-6648
DOCUMENT TYPE: Journal
LANGUAGE: Italian
IT **23934-69-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23934-69-2 HCAPLUS
CN 1-Propanone, 3-[(diphenylmethyl)amino]-1-(2-thienyl)- (8CI) (CA INDEX NAME)



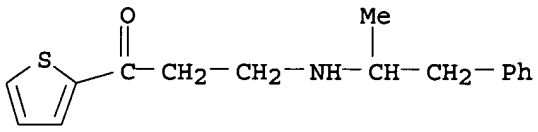
L4 ANSWER 46 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
AB N-(ω-Arylalkyl)dialkylamines, RAr(CH2)nNR1R2, where R is a phenyl or naphthyl group, 2-thienyl, or 2-furyl, are prepared Thus, 15.1 g. 3-phenyl-3-hydroxypropylamine is treated with 14.5 g. PhCH2COMe and the product treated with 1.5 g. NaBH4 to give 25 g. N-(3-phenyl-3-hydroxypropyl)-N-(1-methyl-2-phenylethyl)amine-HCl (I), m. 158-60°. I (25 g.) is treated with 40 ml. SOCl2 to give 30 g. N-(3-phenyl-3-chloropropyl)-N-(1-methyl-2-phenylethyl)-amine-HCl (II), m. 152-4°. II (10 g.) is treated with 30-40 ml. C6H6 in the presence of 8 g. AlCl3 to give 12 g. N-(3,3-diphenylpropyl)-N-(1-methyl-2-phenylethyl)amine-HCl, m. 190-2°, (MeOH). Also prepared are (m.p. given): N-(3,3-diphenylpropyl)dimethylamine-HCl, 186-8°; N-(3,3-diphenylpropyl)-diethylamine-HCl, 172-4°; N-(3,3-diphenylpropyl)dipropylamine-HCl, 146-8°; N-(3,3-diphenylpropyl)dibutylamine-HCl, 120-2°; N-(3,3-diphenylpropyl)morpholine-HCl, 202-4°; N-[3-phenyl-3-(p-tolyl)propyl]dimethylamine-HCl, 182-4°; N-[3-phenyl-3-(3,4-dimethylphenyl)propyl]dimethylamine-HCl, 178-80°; N-[3-phenyl-3-(2,4-dimethylphenyl)propyl]dimethylamine-HCl, 184-6°; N-[3-(p-tolyl)-3-(2,4-dimethylphenyl)propyl]dimethylamine-HCl, 138-40°; N-[3-phenyl-3-(p-fluorophenyl)propyl]dimethylamine-HCl, 180-2°; N-[3-propyl-3-(p-tolyl)propyl]diethylamine-HCl, 156-8°; N-[3-phenyl-3-(p-fluorophenyl)propyl]diethylamine-HCl, 138-40°; N-[3-phenyl-3-(p-fluorophenyl)propyl]piperidine-HCl, 158-60°; N-[3-(p-tolyl)-3-(p-fluorophenyl)propyl)piperidine-HCl, 140-2°; N-[3-phenyl-3-(p-fluorophenyl)propyl]pyrrolidine-HCl, 159-61°; N-[3-phenyl-3-(p-fluorophenyl)propyl]morpholine-HCl, 198-200°; N-[3-(p-tolyl)-3-(p-fluorophenyl)propyl]morpholine-HCl 180-2°; N-[3,3-diphenylpropyl]-1-azacycloheptane-HCl, 190-2°; N-[3-phenyl-3-(p-tolyl)propyl]-1-azacycloheptane-HCl, 184-6°; N-[3-phenyl-3-(p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 206-8°; N-[3-phenyl-3-(p-tolyl)propyl]-N-(2-phenyl-1-methylethylamine-HCl, 178-80°; N-[3-(p-ethylchlorophenyl)-3-(p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 200-2°. N-[3-(p-tolyl)-3-(p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 176-8°; N - [3-phenyl-3-(3,4-dimethylphenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 176-8°; N-[3-phenyl-3-(2,4-dimethylphenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 165-7°; N-[3-(p-fluorophenyl)-3-(p-tolyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 206-8°; N-(3,3-dimethylphenyl)-N-(2-phenyl-1-methylethyl)-N-methylamine-HCl, 168-70°; N-[3-(p-tolyl)-3-phenylpropyl]-N-(2-phenyl-1-methylethyl)-N-methylamine-HCl, 140-2°; N-[3,3-di(p-tolyl)propyl]-N-(2-phenyl-1-methylethyl)-N-methylamine-HCl, 141-3°; N-[3-phenyl-3-(p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)-N-methylamine-HCl, 164-6°; N-[3-(p-chlorophenyl)-3-(methyl-p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 170-2°; N-(3,3-diphenylpropyl)-N-(1-phenylethyl)amine-HCl, 204° and 205°; N-[3-phenyl-3-(p-tolyl)propyl]-N-(1-phenylethyl)amine-HCl, 196-8°; N-(3-m-tolyl)-3(p-tolyl)propyl]-N-(1-phenylethyl)amine-HCl, 188-90°; N-[3-phenyl-3-(p-fluorophenyl)propyl]-N-(1-phenylethyl)amine-HCl, 206-8°; N-(3,3-diphenylpropyl)-N-(1-phenylpropyl)amine-HCl, 214-16°;

N-[3-phenyl-3-(p-fluorophenyl)propyl]-N-(1-phenylpropyl)amine-HCl, 218-20°; N-(3-phenyl-3-(p-tolyl)propyl]-N-(1-phenylpropyl)-amine-HCl, 208-10°; N-[3-(m-tolyl)-3-(p-tolyl)propyl]-N-(1-phenylpropyl)amine-HCl, 188-90°; N-[2,2-diphenylethyl]dimethylamine-HCl, 203-5°; N-[2-phenyl-2-(p-fluorophenyl)-ethyl]dimethylamine-HCl, 208-10°; N - (2,2-diphenylethyl)-diethylamine-HCl, 116-18°; N - (2,2-diphenylethyl)piperidine-HCl, 180-2°; amine maleate m. 140-2°; N-(2,2-diphenylethyl)morpholine-HCl, 211-13°; N-[2-phenyl-2-(p-fluorophenyl)ethyl]piperidine-HCl, 178-80°; amine maleate m. 152-4°; N-[2-phenyl-2-(p-fluorophenyl)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 160-2°; N-(2-phenyl-2-(p-tolyl)-ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 168-70°; N-[2-(m-tolyl)-2-(p-tolyl)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 156-8°; N-[2-(0-tolyl)-2-(p-tolyl)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 152-4°; N-[2-phenyl-2-(p-chlorophenyl)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 163-5°; N-(2,2-diphenylethyl)-N-methyl-N-(2-phenyl-1-methyl-ethyl)amine maleate, 134-6°; N-[2-phenyl-2-(p-fluorophenyl)-ethyl]-N-methyl-N-(2-phenyl-1-methylethyl)amine maleate, 140-2°; N-[2-phenyl-2-(p-tolyl)ethyl]-N-methyl-N-(2-phenyl-1-methylethyl)amine maleate, 146-8°; N-(2,2-diphenylethyl)-N-(1-phenylethyl)amine maleate, 138-40°; N-[2-phenyl-2-(p-fluorophenyl)ethyl]-N-(1-phenylethyl)amine maleate, 130-2°; N-[2-phenyl-2-(p-tolyl)ethyl]-N-(1-phenylethyl)amine maleate, 128-30°; N-[2-(m-tolyl)-2-(p-tolyl)ethyl]-N-(1-phenylethyl)-amine maleate, 128-30°; N-(2,2-diphenylethyl)-N-(1-phenylethyl]-amine maleate, 133-5°; N-[2-phenyl-2-(p-fluorophenyl)-ethyl]-N-(1-phenylpropyl)amine maleate, 130-2°; N-(2,2-diphenylethyl)-N-benzylamine-HCl, 210-12°; N-[2-phenyl-2-(p-tolyl)ethyl]-N-benzylamine-HCl, 203-5°; α-N-(3,3-diphenyl-propyl)morpholine-HCl, 196-8°.; β-N-(3,3-diphenylpropyl)morpholine-HCl,190-2°; N-[3-phenyl-3-(2-thienyl)propyl]dimethyl-amine-HCl, 132-4°; N-[3-phenyl-3-(2-thienyl)propyl]diethyl-amine-HCl, 123-5°; N-[2-phenyl-2-(2-thienyl)ethyl]diethyl-amine-HCl, 128-30°; N-[3-phenyl-3-(2-thienyl)propyl]piperidine maleate, 118-20°; N-[3-phenyl-3-(2-thienyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 178-80°; N-[2-phenyl-2-(2-thienyl)ethyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 144-6°; N-[3-phenyl-3-(2-furyl)propyl]dimethylamine maleate, 134-6°; N-[3-phenyl-3-(2-furyl)propyl]diethylamine maleate, 130-2°; N-[2-phenyl-2-(2-furyl)ethyl]diethylamine maleate, 122-4°; N-[3-phenyl-3-(2-furyl)propyl]piperidine maleate, 128-30°; N-[2-phenyl-2-(2-furyl)ethyl]morpholine maleate, 136-8°; N-[3-phenyl-3-(2-furyl)propyl]-N-(2-phenyl-1-methylethyl)-amine maleate, 124-6°; N-[2-phenyl-2-(2-fury)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 118-20°; N-[3-phenyl-3-(1-naphthyl)propyl]dimethylamine-HCl, 154-6°, amine picrate m. 166-8°; N-[3-phenyl-3-(1-naphthyl)propyl]diethylamine-HCl, 138-40°, amine picrate m. 150-2°; N-[2-phenyl-2-(1-naphthyl)ethyl]diethylamine-HCl, 130-2°; N-[3-phenyl-3-(1-naphthyl)propyl]piperidine-HCl, 128-30°; N-[2-phenyl-2-(1-naphthyl)ethyl]morpholine-HCl, 154-6°; N-[3-phenyl-3-(1-naphthyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 188-90°; N-[3-phenyl-3-(2-naphthyl)propyl]dimethylamine-HCl, 140-2°; N-[3-phenyl-3-(2-naphthyl)propyl]diethylamine-HCl, 136-8°; N-[3-phenyl-3-(2-naphthyl)propyl]piperidine maleate, 128-30°; N-[3-phenyl-3-(5,6,7,8-tetrahydro-1-naphthyl)propyl]diethyl-amine-HCl, 98-110°; N-[2-phenyl-2-(5,6,7,8-tetrahydro-1-naphthyl)ethyl]diethylamine-HCl, 10° (-108°) [sic]; N-[3-phenyl-3-(5,6,7,8-tetrahydro-1-naphthyl)propyl]piperidine maleate,

112-14°; N-[2-phenyl-2-(5,6,7,8-tetrahydro-1-naphthyl)ethyl]-piperidine maleate, 118-20°; N-[2-phenyl-2-(5,6,7,8-tetrahydro-1-naphthyl)ethyl]morpholine-HCl, 110-12°; N-[3-phenyl-3-(5,6,7,8-tetrahydro-1-naphthyl)ethyl]morpholine-HCl, 104-6°; N-[3-phenyl-3-(5,6,7,8-tetrahydro)propyl] - N - (2-phenyl-1-methylethyl)amine-HCl, 160° (turbid) and 182-4°; N-[3-phenyl-3-(2-naphthyl)propyl]-N-(2-phenyl-1-methylethyl)-amine-HCl, 140-2°; N-[3-hydroxy-3-(2-thienyl)propyl]dimethyl-amine, 69-71°, HCl salt m. 158-60°; N-[3-chloro-3-(2-thienyl)-propyl]dimethylamine, 42-4°; N-[3-hydroxy-3-(2-thienyl)-propyl]diethylamine, 38-40°; N-[3-hydroxy-3-(2-thienyl)propyl]piperidine-HCl, 160-2°; N-[3-hydroxy-3-(2-thienyl)propyl]-N-(2-phenyl-1-methylethyl)amine, 36-8°, ketone HCl salt m. 164-6°; N-[3-hydroxy-3-(1-naphthyl)propyl]dimethylamine-HCl, 144-6°; N-[3-hydroxy-3-(1-naphythyl)propyl]diethylamine-HCl, 132-4°; N-[3-hydroxy-3-(1-naphthyl)propyl]piperidine, 112-14°; N-[3-chloro-3-(1-naphthyl)propyl]piperidine, 98-100°, HCl salt m. 178-80°; N-[3-hydroxy-3-(1-naphthyl)-propyl]-N-(2-phenyl-1-methylethyl)amine, 34-6°; N-[3-chloro-3-(1-naphthyl)propyl]-N-(2-phenylpropyl)amine-HCl, 152-4°; N-[3-hydroxy-3-(2-naphthyl)propyl]dimethylamine, 90-2°; N-[3-chloro-3-(2-naphthyl)propyl]dimethylamine-HCl, >240°; N-[3-hydroxy-3-(2-naphthyl)propyl]-N-(2-phenyl-1-methylethyl)-amine-HCl, 170-2°, ketone HCl salt m. 158-60°; N-[3-chloro-3-(2-naphthyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 154-6°; 3-phenyl-3-chloropropylamine-HCl, 110-12°; 3,3-diphenylpropylamine-HCl, 204-6°; N-(3-hydroxy-3-phenylpropyl)piperidine, 54-6°; N-(3-phenyl-3-chloropropyl)piperidine-HCl, N-(3,3-diphenylpropyl)piperidine-HCl, 208-10°; N-(2,2-diphenylethyl)-N-(2-phenyl-1-methylethyl)amine, 168-70°; N-[2-phenyl-2-(p-toly)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 166-8°; N-[N-hydroxy-3-(2-naphthyl)propyl]diethylamine, 34-6°; N-[3-chloro-3-(2-naphthyl)propyl]piperidine, 80-2°; N-[3-chloro-3-(2-naphthyl)propyl]piperidine-HCl, >250°.

ACCESSION NUMBER: 1967:46160 HCAPLUS
DOCUMENT NUMBER: 66:46160
TITLE: New method for preparation of diaryl alkyl amines
AUTHOR(S): Klosa, Josef
CORPORATE SOURCE: Privatlab., Berlin-Zehlendorf, Germany
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1966), 34(5-6), 312-34
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: German

IT **13732-63-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 13732-63-3 HCAPLUS
CN 1-Propanone, 3-[(α-methylphenethyl)amino]-1-(2-thienyl)-, hydrochloride (8CI) (CA INDEX NAME)

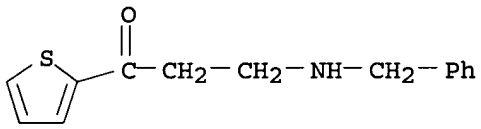


● HCl

L4 ANSWER 47 OF 47 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB A group of ketonic Mannich bases was synthesized by means of the Mannich reaction for pharmacol. study. Some of these bases were reduced with (iso-PrO)3Al (I) to nitrophenyl amino alcohols for use as side chains in future studies. Other bases were brominated to give ketonic nitrogen mustards for study against cancer. Except for appreciable in vitro antituberculous activity of some of the bases, the compds. gave no noteworthy pharmacol. results. The method of Maxwell [Organic Syntheses, Collective Volume III, 305(1955)] was used to prepare the following R'C6H4COCH2CH2NR2 (all as HCl salts, except where otherwise noted) (R', NR2, % yield, m.p. given): p-Cl, NMe2, 71, 176°; p-Cl, NEt2, 60, 145°; p-Cl, piperidino, 56, 190° (HBr salt, m. 205°); p-Br, piperidino, 42, 188° (HBr salt); p-Br, 1-pyrrolidyl, 69, 199°; p-MeO, NMe2, 75, 181° (HBr salt, m. 182°); p-MeO, 1-pyrrolidyl, 38, 184°; p-MeO, NHCH2Ph, 29, 183°; m-MeO, NMe2, 81, 168°; p-HO, NMe2, 56, 192°; m-HO, NMe2, 50, 180°; o-HO, NMe2, 33, 156°; p-Ph, NMe2, 69, 192°; p-O2N, NMe2, 72, 191°; p-O2N, NEt2, 66, 150°; p-O2N, 1-pyrrolidyl, 61, 185°; p-O2N, piperidino, 51, 200° (HBr salt, m. 189°); p-O2N, NPr2, 26, 140°; p-O2N, N(CH2CH2OH)2, 19, 146°; p-O2N, morpholino, 62, 218°; m-O2N, 1-pyrrolidyl, 63, 182°; m-O2N, piperidino, -, 180°. The following compds. were prepared similarly: 2-(β-1-pyrrolidylpropionyl)thiophene HCl salt, m. 169-70°; 2-(β-benzylaminopropionyl)thiophene HCl salt, m. 174-5°; PhCH:CHCOCH2CH2N.CH2.CH2.O.CH2.CH2, m. 178°; PhCH:CHCOCH2CH2N.CH2.CH2.CH2.CH2, m. 178°; 2,3-(MeO)2C6H3CH:CHCOCH2CH2N.CH2.CH2.CH2.CH2, m. 155°; 4-O2NC6H4CH:CHCOCH2CH2N.CH2.CH2.CH2.CH2, m. 196°. To a hot slurry of 20 g. I and 3.3 g. anhydrous AlCl3 in 175 ml. Me2CHOH (II) was added 4-O2NC6H4CH:CHCOCH2CH2NMe2, the mixture brought to full reflux, maintained 15 min. at that temperature, the condenser turned downward for distillation, stirring and removal of Me2CO continued for 2 hrs. (until a neg. test for Me2CO was obtained in the distillate), the condenser reinserted upright, refluxed 10 min., the condenser turned downward for distillation, and a few drops of distillate collected in which a neg. test for Me2CO was obtained; the residual II was removed in vacuo, the residue cooled, treated with 200 ml. ice-cold 10% HCl, the suspension dissolved in 375 ml. H2O, the solution made strongly basic with 40% KOH with cooling and stirring, extracted with Et2O, the extract washed with saturated NaCl solution, dried overnight with Na2SO4, filtered, treated with anhydrous HCl, the resulting oil kept 48 hrs. in the refrigerator, the resulting solid filtered off, and washed with cold Me2CO to give 10.4 g. 4-O2NC6H4CH:CHCH(OH)CH2CH2NMe2.HCl, m. 180-1°. The following R'C6H4CH(OH)CH2CH2NR2.HCl were similarly prepared (R', NR2, %

yield, m.p. given): H, NMe2, 65, 134°; p-O2N, NMe2, 65, 176°; p-O2N, NEt2, 54, 140°; p-O2N, 1-pyrrolidyl, 61, 168°; p-O2N, piperidino, 55, 177°; p-O2N, 4-morpholino, 67, 185°; m-O2N, NMe2, 42, 188°. Bromination of the appropriate ketonic base-HBr salts in AcOH (method of Land, et al., C.A. 41, 2038b) gave the following 4-R'C6H4COCHBrCH2NR2 (all as HBr salts except where otherwise noted) (R', NR2, % yield, m.p. given): H, piperidino, 85, 185°; H, morpholino, 85, 181°; Cl, NMe2, 78, 191° (HCl salt); Cl, piperidino, 82, 175°; Br, NEt2, 80, 150°; Br, piperidino, 81, 168°; MeO, NMe2, 86, 169°; MeO, piperidino, 87, 145°; O2N, piperidino, 84, 182°.

ACCESSION NUMBER: 1958:61218 HCAPLUS
DOCUMENT NUMBER: 52:61218
ORIGINAL REFERENCE NO.: 52:11067a-i
TITLE: Ketonic Mannich bases and the products of their reduction and bromination
AUTHOR(S): Nobles, Lewis W.; Burckhalter, J. H.
CORPORATE SOURCE: Univ. of Kansas, Lawrence
SOURCE: Journal of the American Pharmaceutical Association, Scientific Edition (1958), 67, 77-81
CODEN: JAPMA8; ISSN: 0095-9553
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:61218
IT **108245-96-1**, 1-Propanone, 3-benzylamino-1-(2-thienyl)-, hydrochloride
(preparation of)
RN 108245-96-1 HCAPLUS
CN 1-Propanone, 3-benzylamino-1-(2-thienyl)-, hydrochloride (6CI) (CA INDEX NAME)



● HCl

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